10/620,520

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PASSWORD:
* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 09:08:22 ON 13 MAY 2006
FILE 'REGISTRY' ENTERED AT 09:08:22 ON 13 MAY 2006
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	3.52	3.73

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	3.96	4.17

FILE 'REGISTRY' ENTERED AT 09:08:57 ON 13 MAY 2006
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STRUCTURE FILE UPDATES: 11 MAY 2006 HIGHEST RN 883943-03-1
DICTIONARY FILE UPDATES: 11 MAY 2006 HIGHEST RN 883943-03-1

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

```
**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005.  A new display format, IDERL, is now     *
* available and contains the CA role and document type information.  *
*                                                                    *
**********************************************************************
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Structure search iteration limits have been increased. See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\09591177b.str

L5 STRUCTURE UPLOADED

=> s l5 sss sam
SAMPLE SEARCH INITIATED 09:09:23 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 21 TO ITERATE

100.0% PROCESSED 21 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

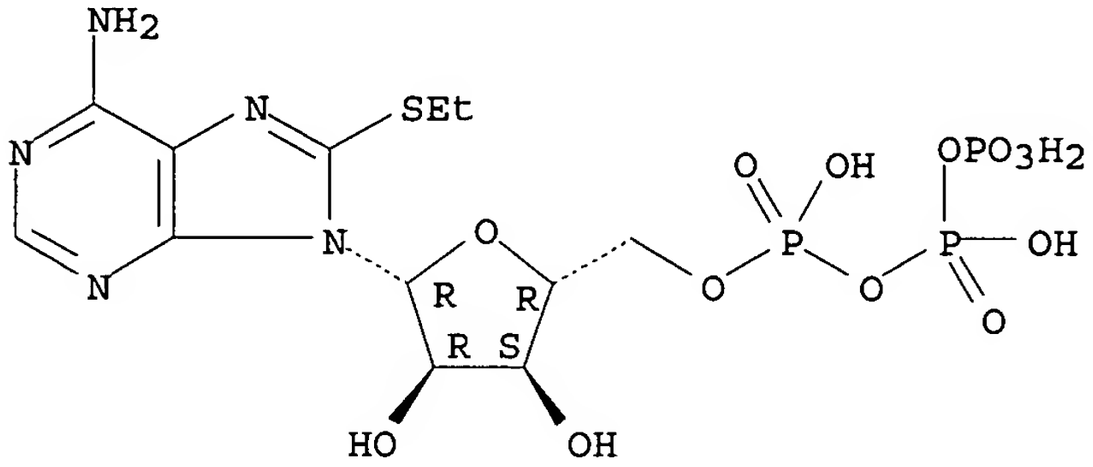
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 146 TO 694
PROJECTED ANSWERS: 2 TO 124

L6 2 SEA SSS SAM L5

=> d scan l6

L6 2 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Adenosine 5'-(tetrahydrogen triphosphate), 8-(ethylthio)- (9CI)
MF C12 H20 N5 O13 P3 S
CI COM

Absolute stereochemistry.

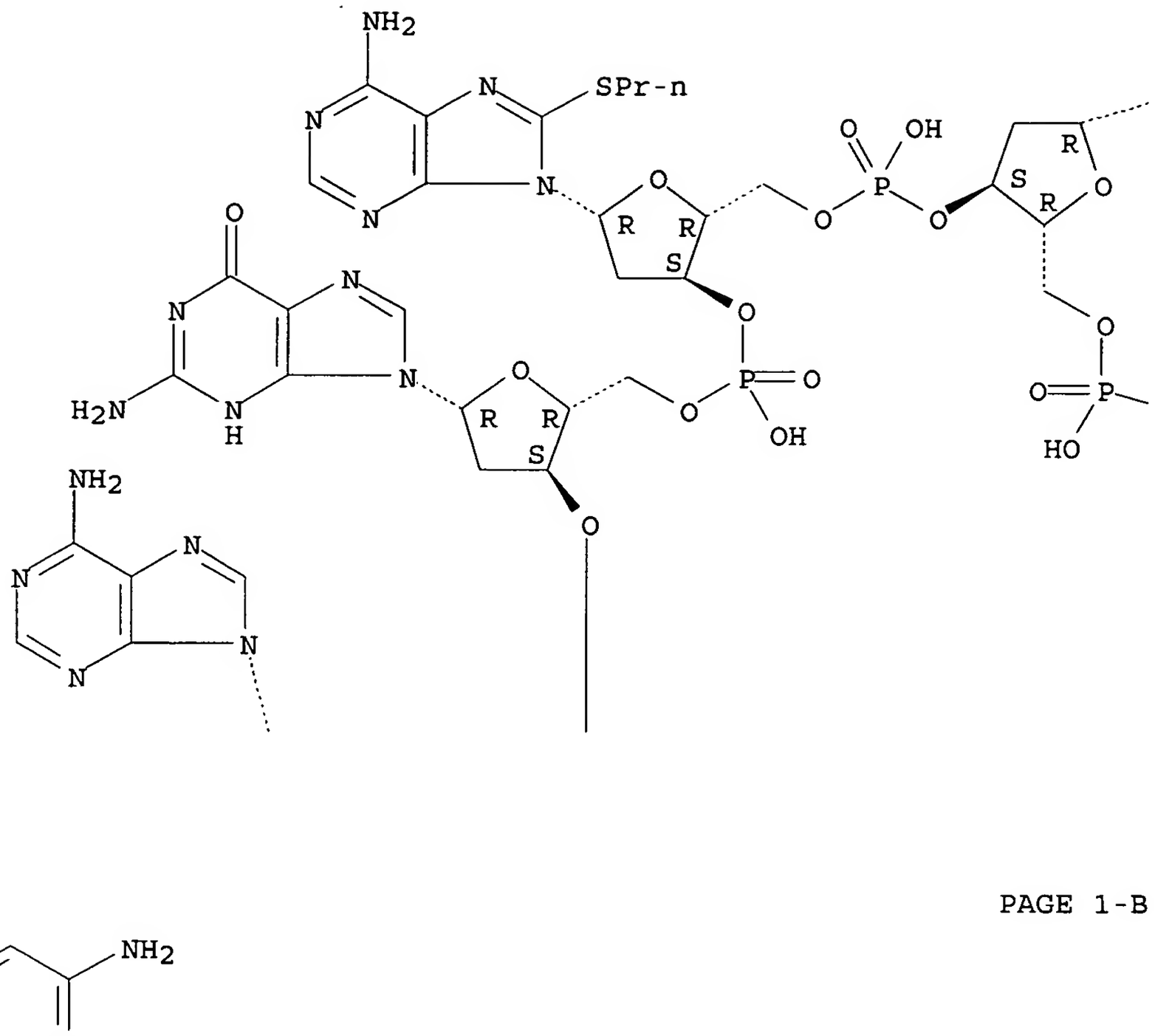


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 2 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Thymidine, 2'-deoxyadenylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-
2'-deoxycytidylyl-(3'→5')-2'-deoxy-8-(propylthio)adenylyl-
(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxyadenylyl-
(3'→5')- (9CI)
MF C72 H92 N30 O38 P6 S

Absolute stereochemistry.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O
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R
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S
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R
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R
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N
O
N
H2N
N
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OH
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HO
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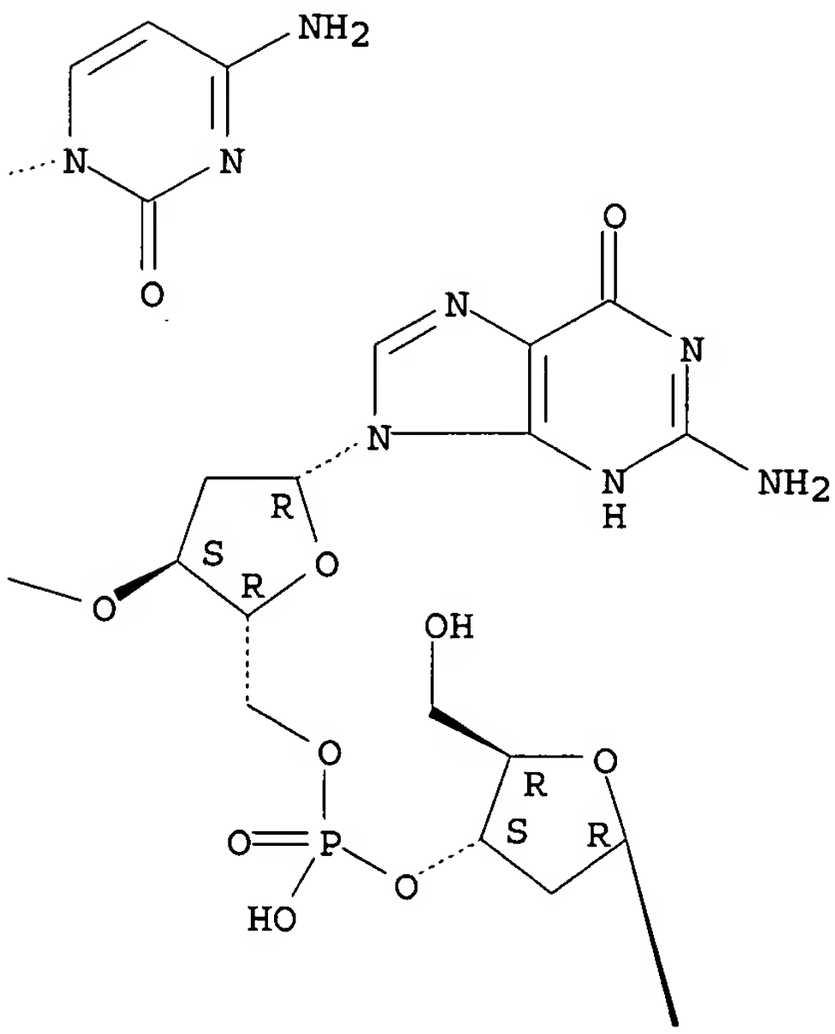
O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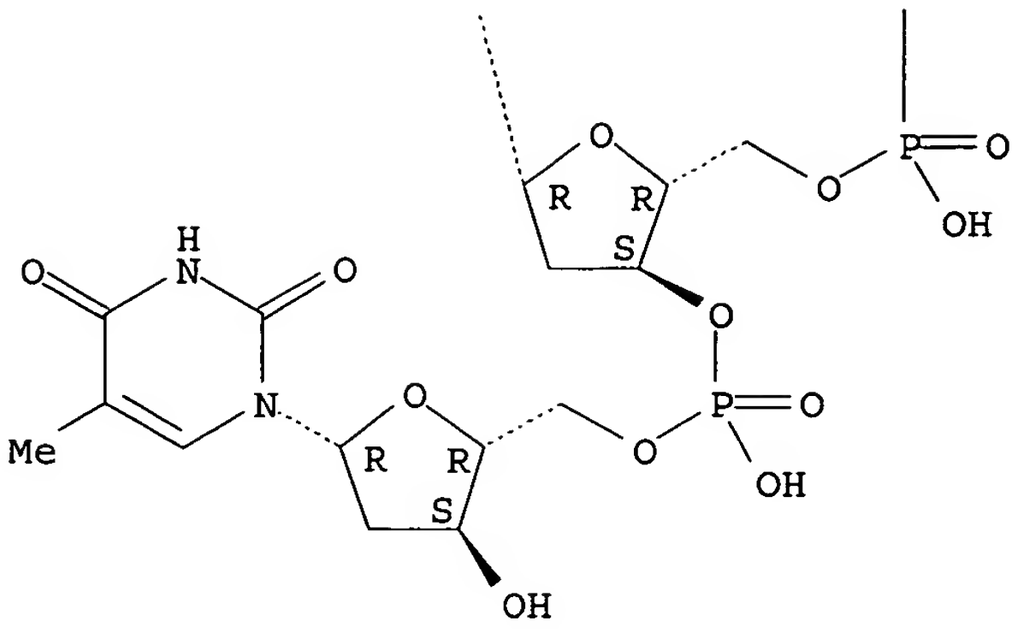
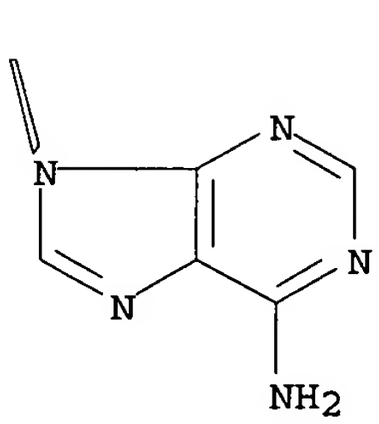
HO





PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s l5 sss full
FULL SEARCH INITIATED 09:10:13 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 351 TO ITERATE

100.0% PROCESSED 351 ITERATIONS 32 ANSWERS
SEARCH TIME: 00.00.01

L7 32 SEA SSS FUL L5

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	167.38	171.55

FILE 'CAPLUS' ENTERED AT 09:10:18 ON 13 MAY 2006
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FILE COVERS 1907 - 13 May 2006 VOL 144 ISS 21
FILE LAST UPDATED: 11 May 2006 (20060511/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
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http://www.cas.org/infopolicy.html

=> s l7
L8 17 L7

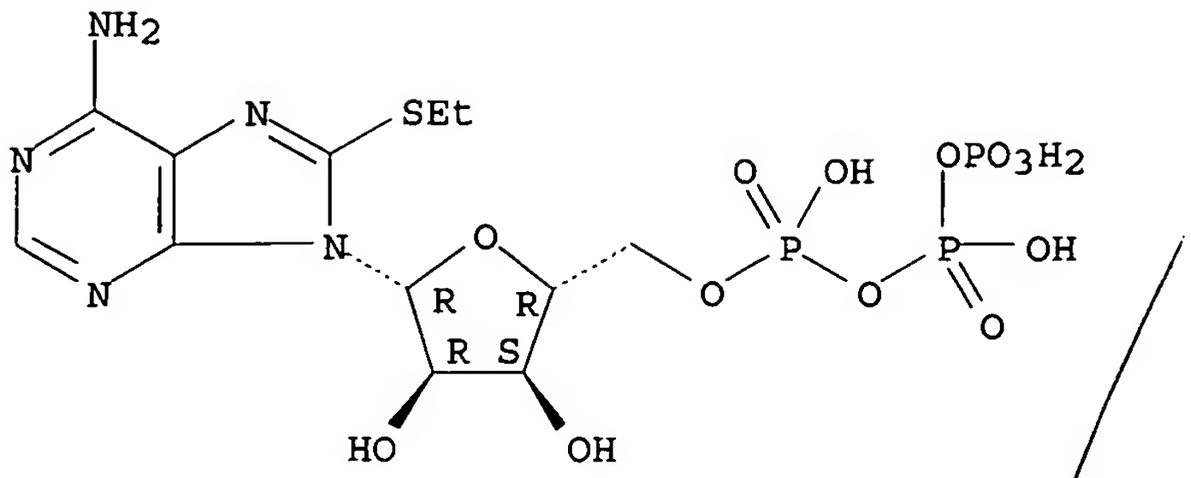
=> d bib abs hitstr 1-17 l8

L8 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:911398 CAPLUS
DN 142:214281
TI C8-substituted purine nucleotide analogs and their use as inhibitors of nucleoside triphosphate diphosphohydrolases
IN Halbfinger, Efrat; Fischer, Bilha; Beaudoin, Adrien R.; Gendron, Fernand Pierre
PA Universite de Sherbrooke, Can.; Bar-Ilan University
SO Can. Pat. Appl., 54 pp.
CODEN: CPXXEB
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI CA 2311084	AA	20011209	CA 2000-2311084	20000609
PRAI CA 2000-2311084		20000609		

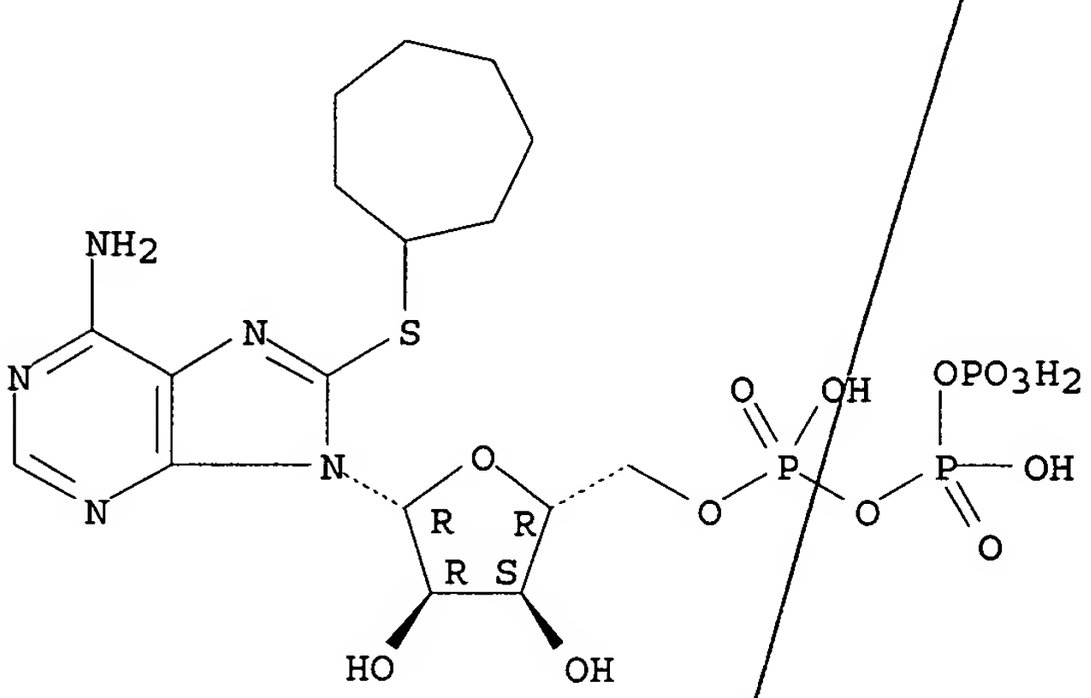
OS CASREACT 142:214281
AB Ectonucleoside triphosphate diphosphohydrolases [NTPDases; EC 3.6.1.5] constitute a family of enzymes which are involved in the metabolism of extracellular nucleotides, catalyzing the hydrolysis of the gamma and beta phosphate bonds of triphospho- and diphosphonucleosides (whereas 5'-nucleotidases [EC 3.1.3.5] catalyze the hydrolysis of alpha phosphate bond of monophosphonucleosides). These extracellular nucleotides interact with endothelial, epithelial and smooth muscle cells, as well as blood cells and lymphoid cells, to influence the different physiol. systems of vertebrates. Since these ecto-nucleotidases alter the extracellular concns. of nucleotides these enzymes modulate their physiol. effects, including, for example, platelet aggregation, heart function, control of vascular tone and inflammation reactions, electrolyte secretion and gastrointestinal motility, neurotransmission both in central and peripheral nervous systems, as well as other effects in other physiol. systems. This invention provides C8 substituted purine nucleotide analogs, such as ATP analogs, and further provides their use as inhibitors of NTPDases and thereby as tools to modulate the conversion of nucleotides into nucleoside derivs., and thus modulate the levels of these compds. Such modulation further provides for the modulation of the activity and function of many processes which are affected by these compds.
IT **81609-35-0P 284040-51-3P 284040-52-4P**
284040-53-5P
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(C8-substituted purine nucleotide analogs and their use as inhibitors of nucleoside triphosphate diphosphohydrolases to modulate purine nucleotide levels and biol. processes)
RN 81609-35-0 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(ethylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



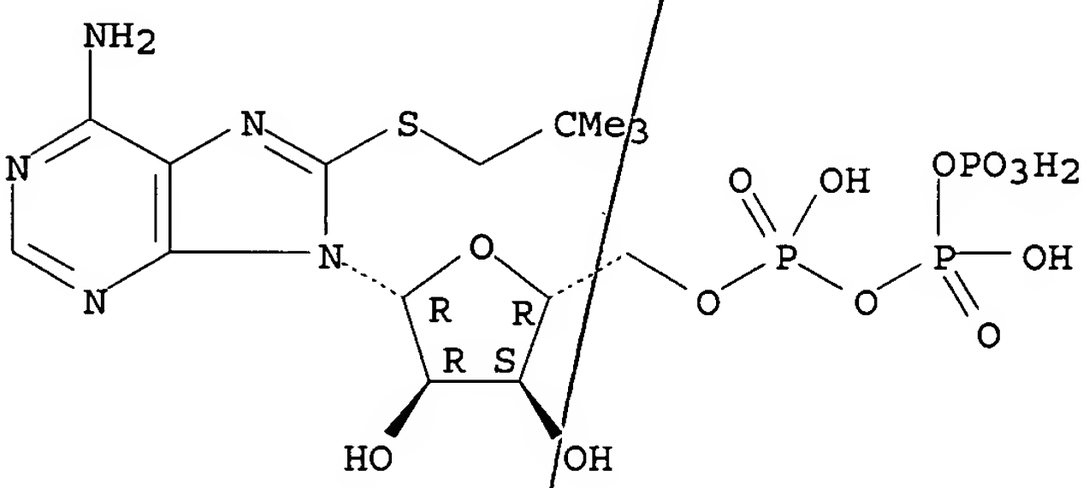
RN 284040-51-3 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(cycloheptylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



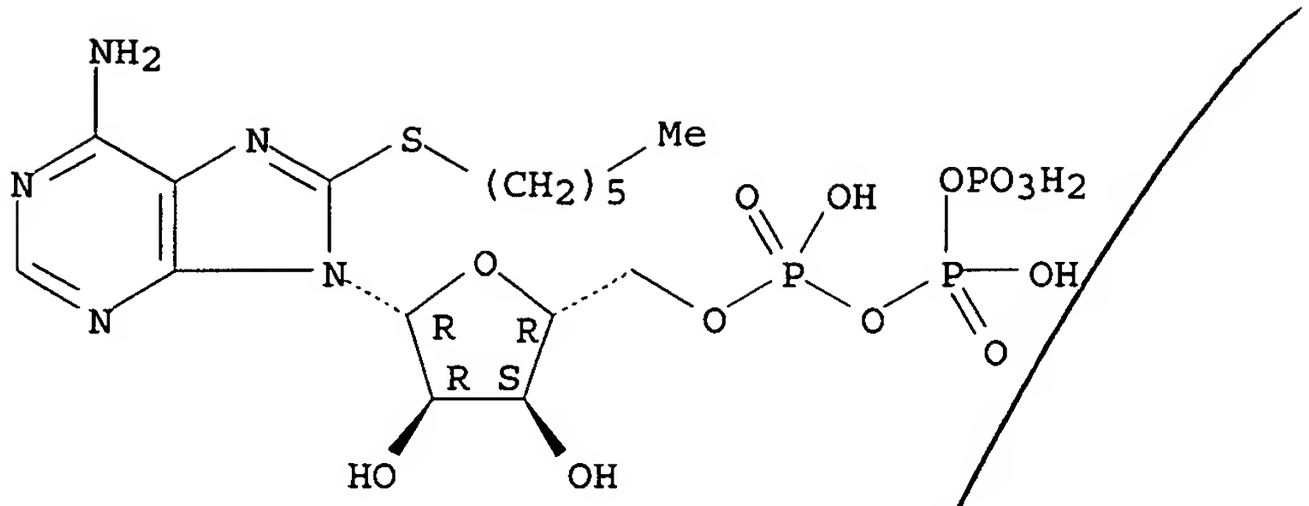
RN 284040-52-4 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-[(2,2-dimethylpropyl)thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



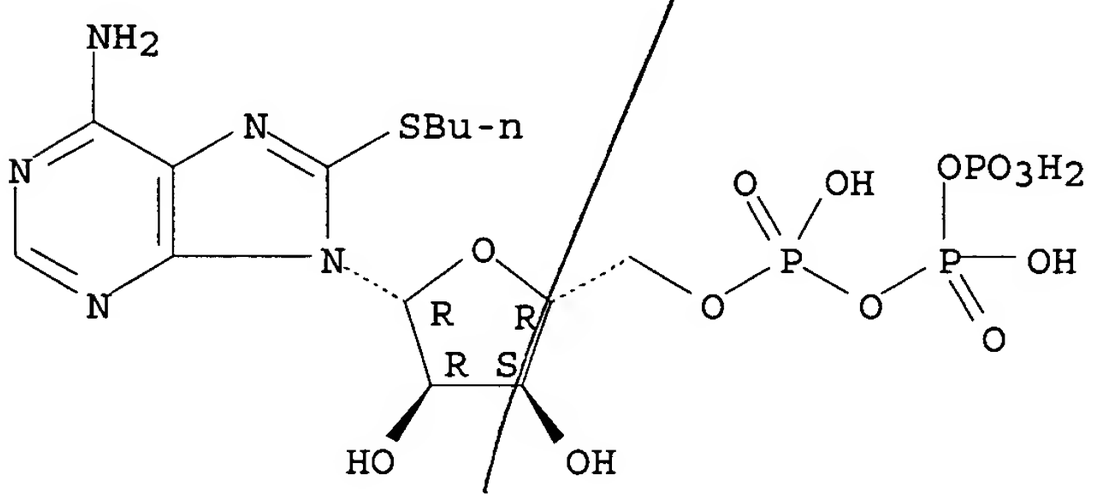
RN 284040-53-5 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(hexylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **284040-54-6**
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(C8-substituted purine nucleotide analogs and their use as inhibitors of nucleoside triphosphate diphosphohydrolases to modulate purine nucleotide levels and biol. processes)
RN 284040-54-6 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:617808 CAPLUS
DN 141:270997
TI Molecular Recognition in Purinergic Receptors. 1. A Comprehensive Computational Study of the h-P2Y1-Receptor
AU Major, Dan T.; Fischer, Bilha
CS Gonda-Goldschmied Medical Research Center, Department of Chemistry, Bar-Ilan University, Ramat-Gan, 52900, Israel
SO Journal of Medicinal Chemistry (2004), 47(18), 4391-4404
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB P2Y receptors (P2Y-Rs) are attractive pharmaceutical targets due to their involvement in the modulation of many tissues and organs. The lack of exptl. structural data on P2Y-Rs impedes structure-based drug design. The need to elucidate the receptor's mol. recognition, together with the limitations of previous receptor models, triggered the construction of a new mol. model for the h-P2Y1-R. Therefore, a h-P2Y1-R model was constructed by homol. modeling using the 2.6 Å crystal structure of bovine rhodopsin as a template and subsequently refined by constrained mol. dynamics (MD) simulations in a fully hydrated lipid bilayer environment. ATP was docked into the receptor binding site, followed by binding site refinement using Monte Carlo and MD simulations. Anal. of the h-P2Y1-R-ATP complex suggests that the triphosphate moiety is tightly bound by a multitude of interactions possibly including a Mg2+ ion, the ribose ring is not involved in specific interactions, and the adenine ring is bound via N1, N7, and N6. The mol. recognition of the h-P2Y1-R was further probed by ATP derivs. modified on the adenine ring, and correlated with EC50 values for these derivs. Anal. of receptor:ligand complexes and

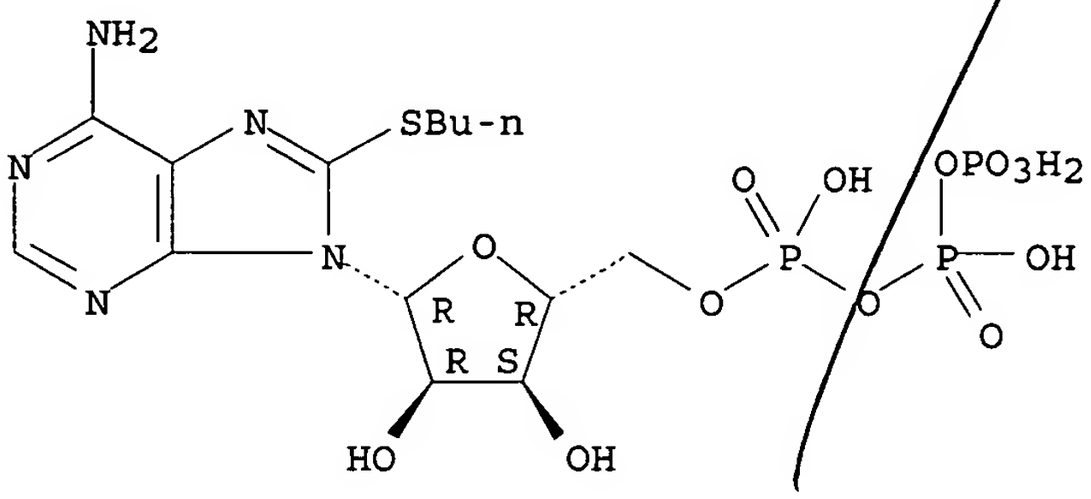
quantum mech. studies on model compds. support the role of both steric and electronic effects in improving H-bonding (via N1 and N6) and π-stacking interactions. The computed h-P2Y1-R model was validated with respect to our previous biochem. results. The authors believe that this new model of the h-P2Y1-R provides the means for understanding phenomena such as the ligand's potency and receptor subtype selectivity.

IT **284040-54-6**
RL: PAC (Pharmacological activity); BIOL (Biological study)
(mol. recognition in human purinergic P2Y1 receptor)

RN 284040-54-6 CAPLUS

CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 71 THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:856092 CAPLUS
DN 139:333119
TI Ecto-nucleoside triphosphate diphosphohydrolase inhibition-based methods for screening for a compound useful in the treatment or prevention of lymphocytic disorders, for inhibiting lymphocyte activity and preventing or treating lymphocytic disorders
IN Beaudoin, Adrien; Benrezzak, Ouhida
PA Bioflash Inc., Can.
SO PCT Int. Appl., 63 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003089664	A1	20031030	WO 2003-CA583	20030422
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2382768	AA	20031019	CA 2002-2382768	20020419
	CA 2479501	AA	20031030	CA 2003-2479501	20030422
	AU 2003226989	A1	20031103	AU 2003-226989	20030422
	US 2005164306	A1	20050728	US 2003-511133	20030422
PRAI	CA 2002-2382768	A	20020419		
	WO 2003-CA583	W	20030422		

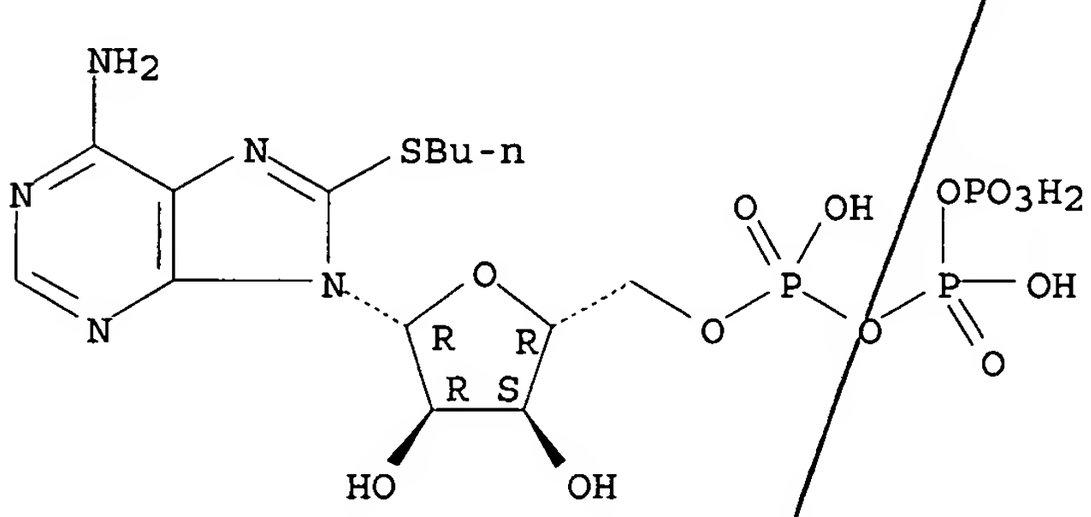
AB The invention discloses a method of screening for a compound useful in the treatment of a disease or condition characterized by an immune cell disorder, wherein the cell expresses ecto-nucleoside triphosphate diphosphohydrolases (NTPDases), the method comprising contacting a candidate compound with NTPDase, wherein the candidate compound is selected if

the activity of the NTPDase is reduced in the presence of the candidate compound as compared to that in the absence thereof. The invention also discloses a method for inhibiting an immune cell activity in a mammal, comprising targeting immune cells with an effective amount of a NTPDase inhibitor. The invention further discloses a method to prevent or reduce the risk of rejection of transplanted tissue or organ, comprising administering to the animal an effective amount of NTPDase inhibitor.

IT **284040-54-6 344402-39-7**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(ecto-nucleoside triphosphate diphosphohydrolase inhibition-based methods for screening for agents for treatment of immune cell disorder-associated conditions)

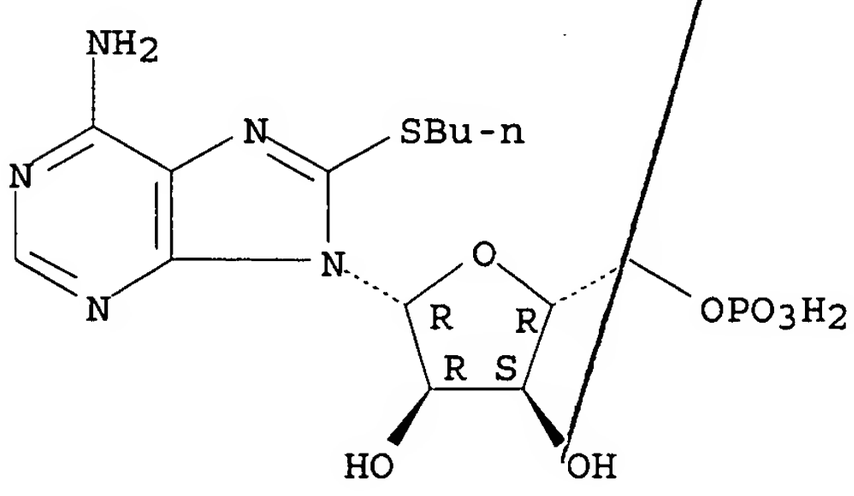
RN 284040-54-6 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 344402-39-7 CAPLUS
CN 5'-Adenylic acid, 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



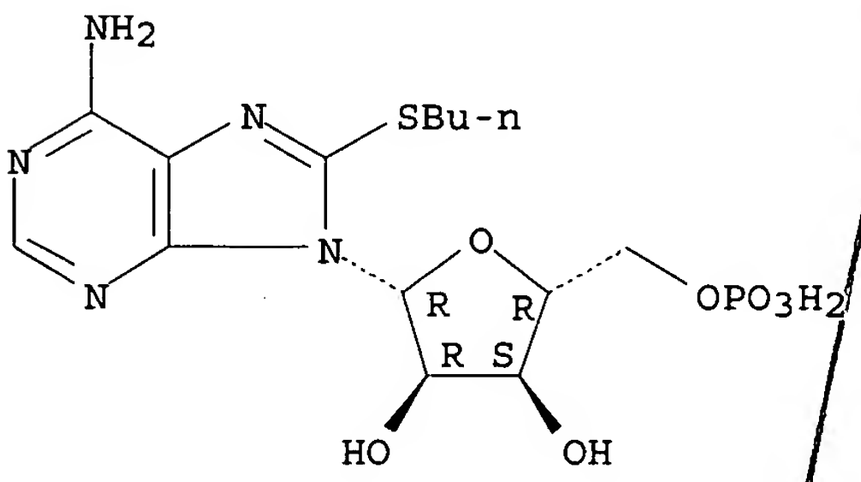
RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:753685 CAPLUS
DN 140:205747
TI Characterization and Elucidation of Coordination Requirements of Adenine Nucleotides Complexes with Fe(II) Ions
AU Richter, Yael; Fischer, Bilha
CS Gonda-Goldschmied Medical Research Center, Department of Chemistry, Bar-Ilan University, Ramat-Gan, Israel
SO Nucleosides, Nucleotides & Nucleic Acids (2003), 22(9), 1757-1780
CODEN: NNNAFY; ISSN: 1525-7770
PB Marcel Dekker, Inc.
DT Journal
LA English
AB In spite of the significant role of iron ions-nucleotide complexes in living cells, these complexes have been studied only to a limited extent. Therefore, we fully characterized the ATP:Fe(II) complex including

stoichiometry, geometry, stability consts., and dependence of Fe(II)-coordination on pH. A 1:1 stoichiometry was established for the ATP:Fe(II) complex based on volumetric titrns., UV and SEM/EDX measurements. The coordination sites of ferrous ions in the complex with ATP, established by 1H-, 31P-, and 15N-NMR, involve the adenine N7 as well as Pα, Pβ, and Pγ. Coordination sites remain the same within the pH range of 3.1-8.3. By applying fluorescence monitored Fe(II)-titration, we established a log K value of 5.13 for the Fe(ATP)2- complex, and 2.31 for the Fe(HATP)- complex. Ferrous complexes of ADP3- and AMP2- were less stable (log K 4.43 and 1.68, resp.). The proposed major structure for the Fe(ATP)2- complex is the open' structure. In the minor closed' structure N7 nitrogen is probably coordinated with Fe(II) through a bridging water mol. The electronic and stereochem. requirements for Fe(II)-coordination with ATP4- were probed using a series of modified-phosphate or modified-adenine ATP analogs. Fe(II) coordinates solely with the phosphate-oxygen atom, and not with sulfur, amine, or borane in the cases of phosphate-modified analogs of ATP. A high electron d. on N7 and an anti conformation of the adenine-nucleotide are required for enhanced stability of ATP analogs:Fe(II) complexes as compared to ATP complexes (up to more than 100-fold). There are no stereochem. preferences for Fe(II)-coordination with either Rp or Sp isomers of ATP-α-S or ATP-α-BH3 analogs.

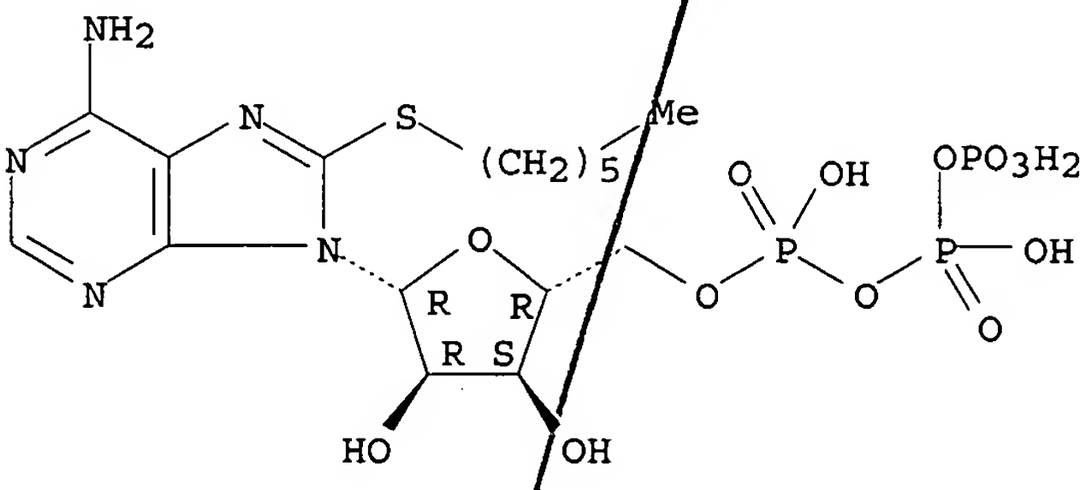
IT **344402-39-7D**, iron aquo complexes
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(iron(2+) coordination with adenine nucleotides)
RN 344402-39-7 CAPLUS
CN 5'-Adenylic acid, 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



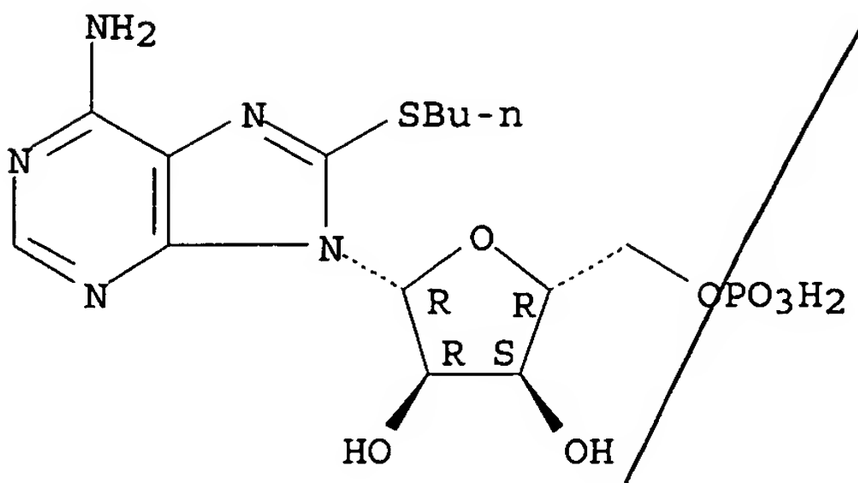
IT **284040-53-5 344402-39-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(iron(2+) coordination with adenine nucleotides)
RN 284040-53-5 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(hexylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 344402-39-7 CAPLUS
CN 5'-Adenylic acid, 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

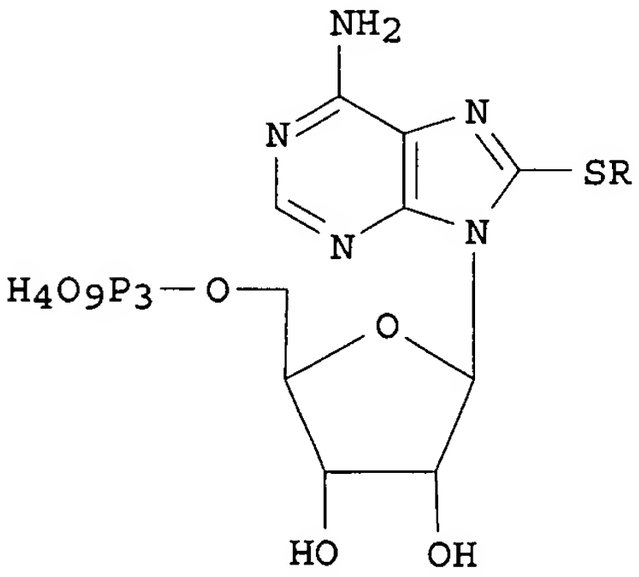


RE.CNT 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:711173 CAPLUS
DN 139:230955
TI Preparation of C8-substituted purine nucleotide analogs as NTPDase inhibitors
IN Beaudoin, Adrien R.; Gendron, Fernand-Pierre; Halbfinger, Efrat; Fischer, Bilha
PA Bar-Ilan University, Israel; Universite De Sherbrooke
SO U.S., 21 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6617439	B1	20030909	US 2000-591177	20000609
US 2004043955	A1	20040304	US 2003-620520	20030716
PRAI US 2000-591177	A3	20000609		

OS MARPAT 139:230955
GI



I

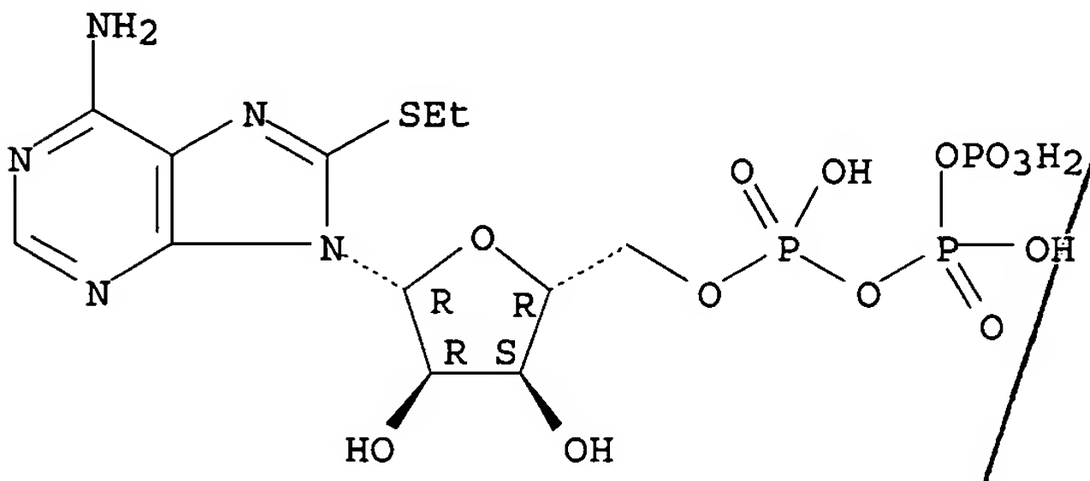
AB C8-substituted purine nucleotide analogs, I (R is alkyl, cycloalkyl) such as ATP analogs, and their use is described, including their use as inhibitors of NTPDases and thereby as tools to modulate the conversion of nucleotides into nucleoside derivs., and thus modulate the levels of these compds. Such modulation further provides for the modulation of the activity and function of many processes which are affected by these compds. Thus, I [R = (CH2)3Me] was prepared and tested in vivo as NTDPase inhibitor. I [R = (CH2)3Me] interacts specifically with the binding site of the enzyme potentially reduces the risk of interference with other ATP-binding enzymes or receptors, and thus possesses a high degree of specificity. The compds. of the invention were analyzed with resp. to any effects on the activity of purinoceptors.

IT **81609-35-0P 284040-51-3P 284040-52-4P**

284040-53-5P 284040-54-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of C8-substituted purine nucleotide analogs as NTPDase inhibitors)

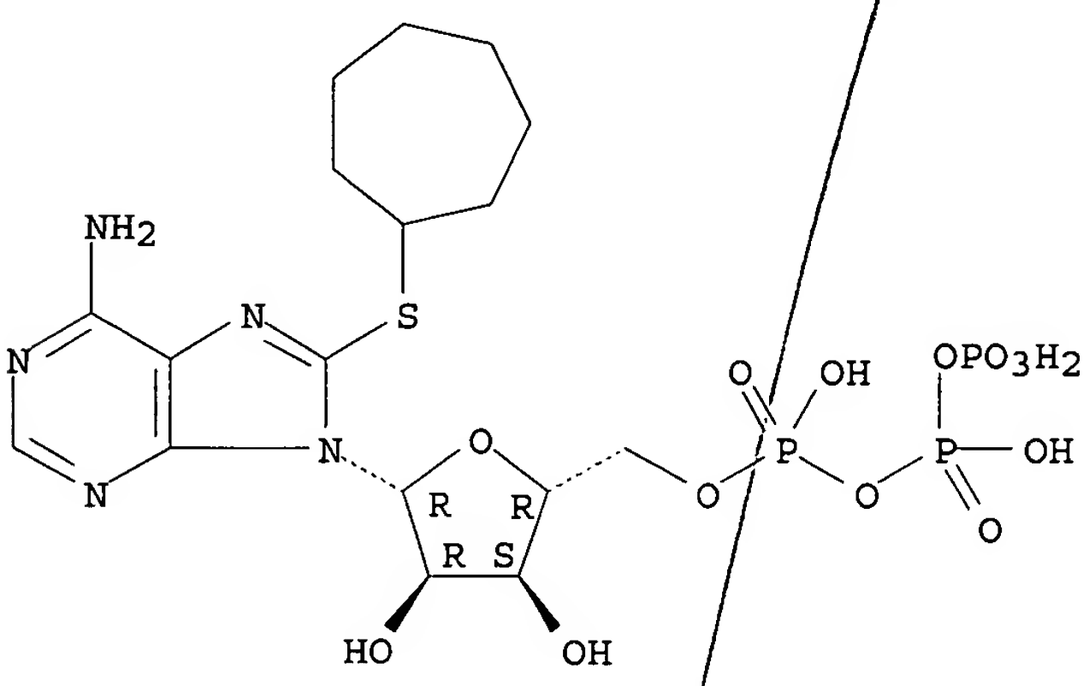
RN 81609-35-0 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(ethylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



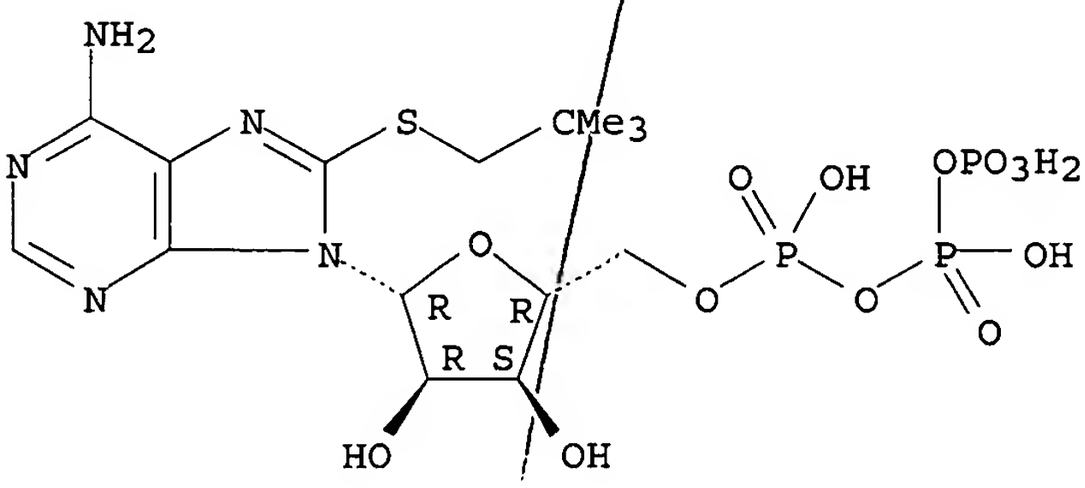
RN 284040-51-3 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(cycloheptylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 284040-52-4 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-[(2,2-dimethylpropyl)thio]- (9CI) (CA INDEX NAME)

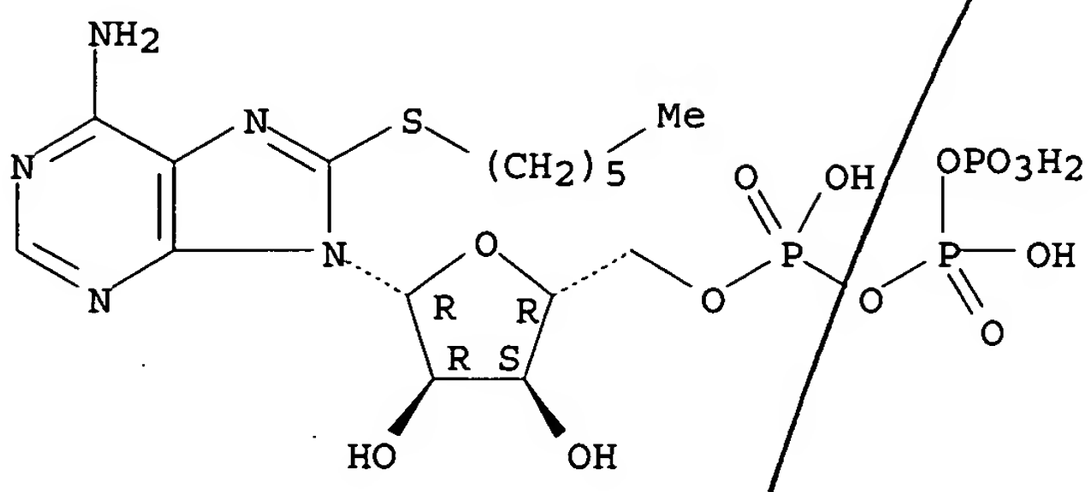
Absolute stereochemistry.



RN 284040-53-5 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(hexylthio)- (9CI) (CA INDEX

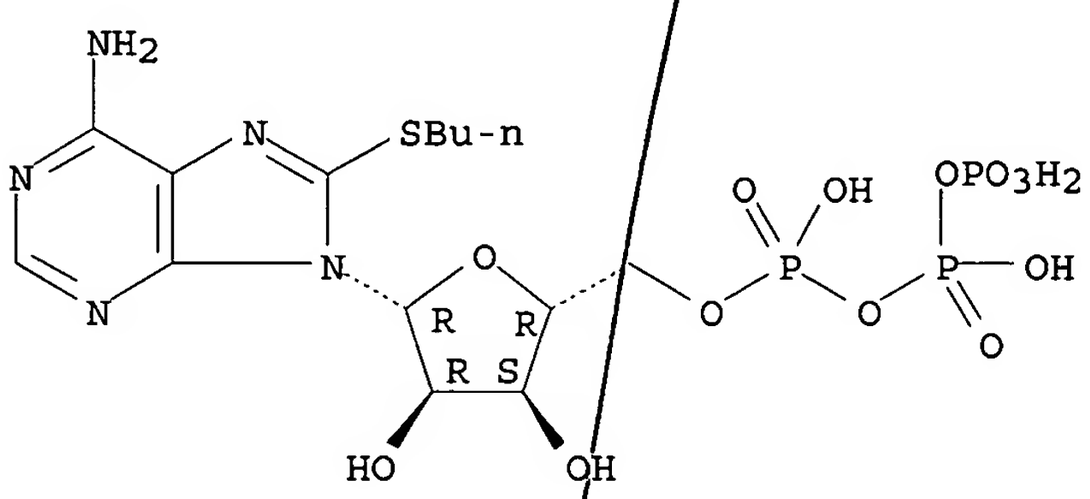
NAME)

Absolute stereochemistry.



RN 284040-54-6 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 71 THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2001:327844 CAPLUS
DN 135:149038
TI Inhibitors of NTPDase: key players in the metabolism of extracellular purines
AU Gendron, F. P.; Halbfinger, E.; Fischer, B.; Beaudoin, A. R.
CS Department of Biology, University of Sherbrooke, Sherbrooke, Can.
SO Advances in Experimental Medicine and Biology (2000), 486(Purine and Pyrimidine Metabolism in Man X), 119-123
CODEN: AEMBAP; ISSN: 0065-2598
PB Kluwer Academic/Plenum Publishers
DT Journal
LA English
AB This study described the potential of a new class of ATP analogs as nucleoside triphosphate diphosphohydrolase (NTPDase) inhibitors. From previous studies, 8-thiobutyladenosine 5'-triphosphate (8-BuS-ATP) appears to be a specific and efficient NTPDase inhibitor. This novel inhibitor is a new tool to regulate NTPDase activity and thereby influencing purine signaling in mammalian.
IT **81609-35-0 284040-51-3 284040-53-5**
284040-54-6
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(inhibitors of nucleoside triphosphate diphosphohydrolase - key players in metabolism of extracellular purines)
RN 81609-35-0 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(ethylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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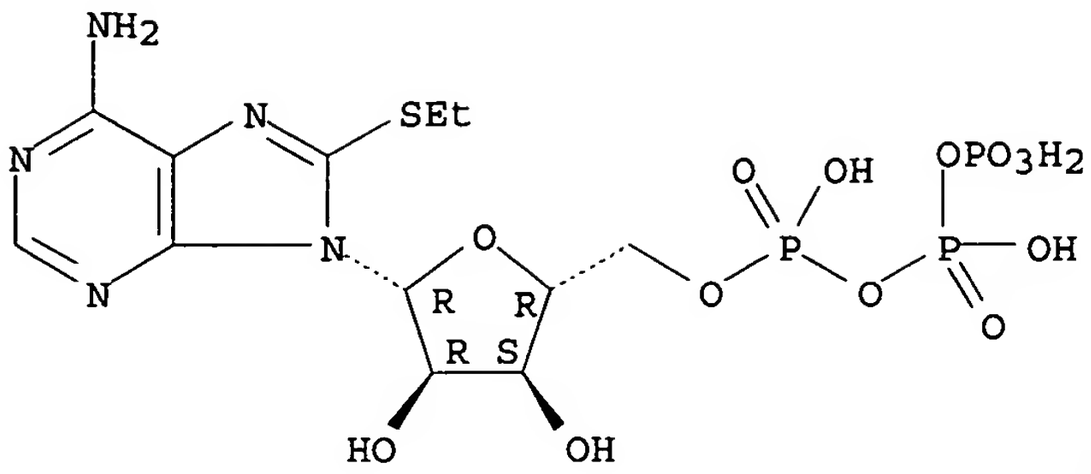
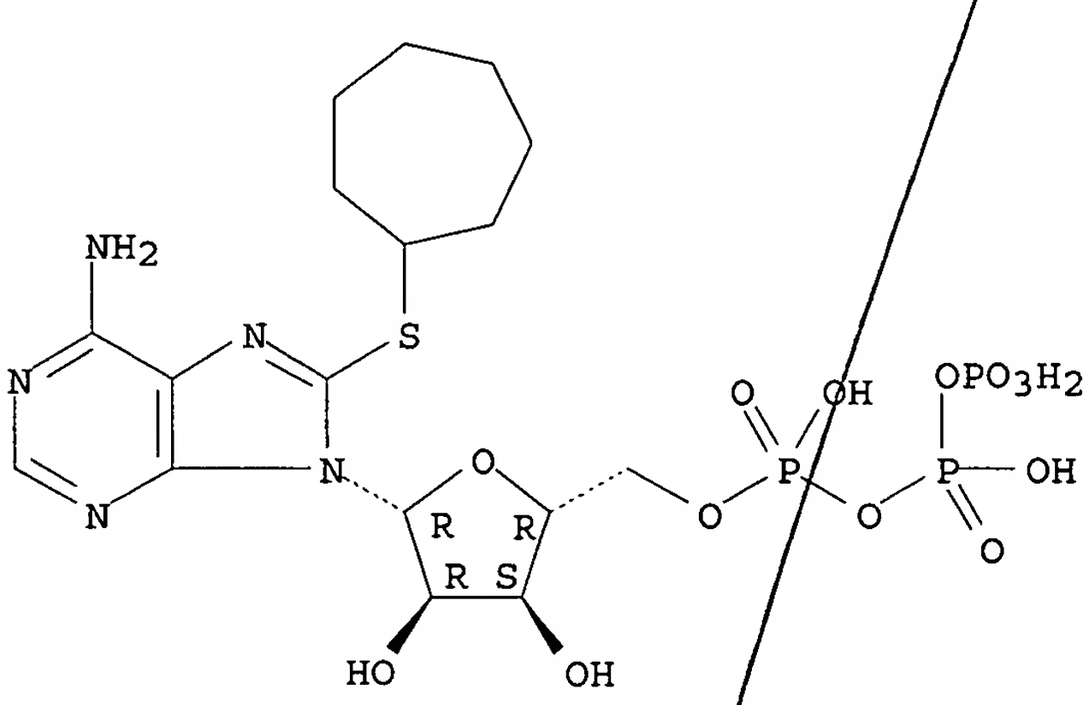


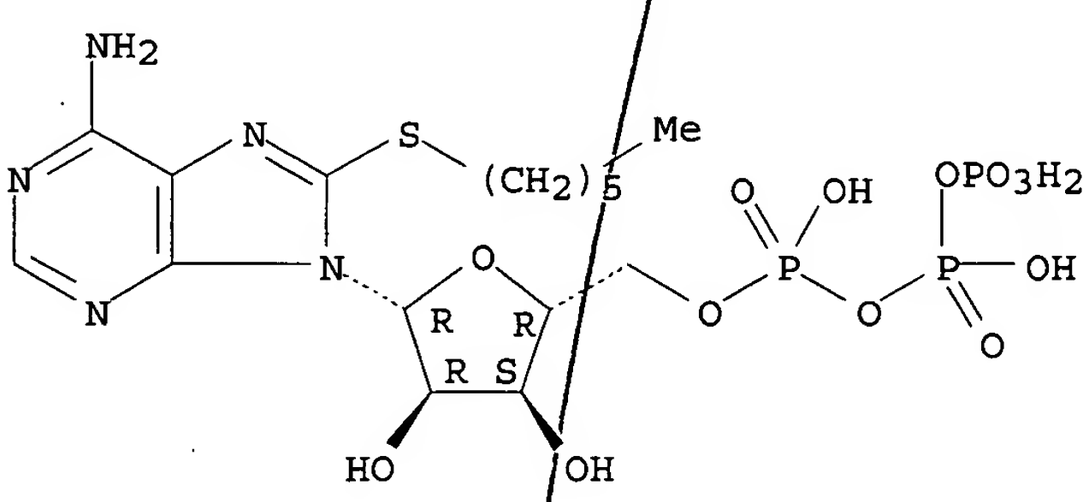
RN 284040-51-3 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(cycloheptylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



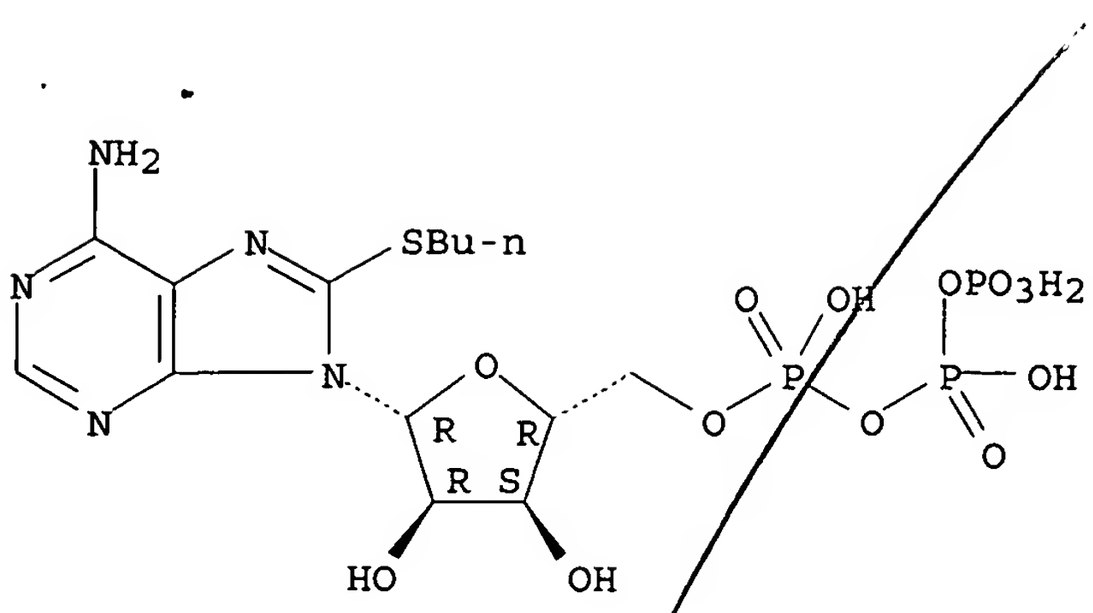
RN 284040-53-5 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(hexylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 284040-54-6 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)- (9CI) (CA INDEX NAME)

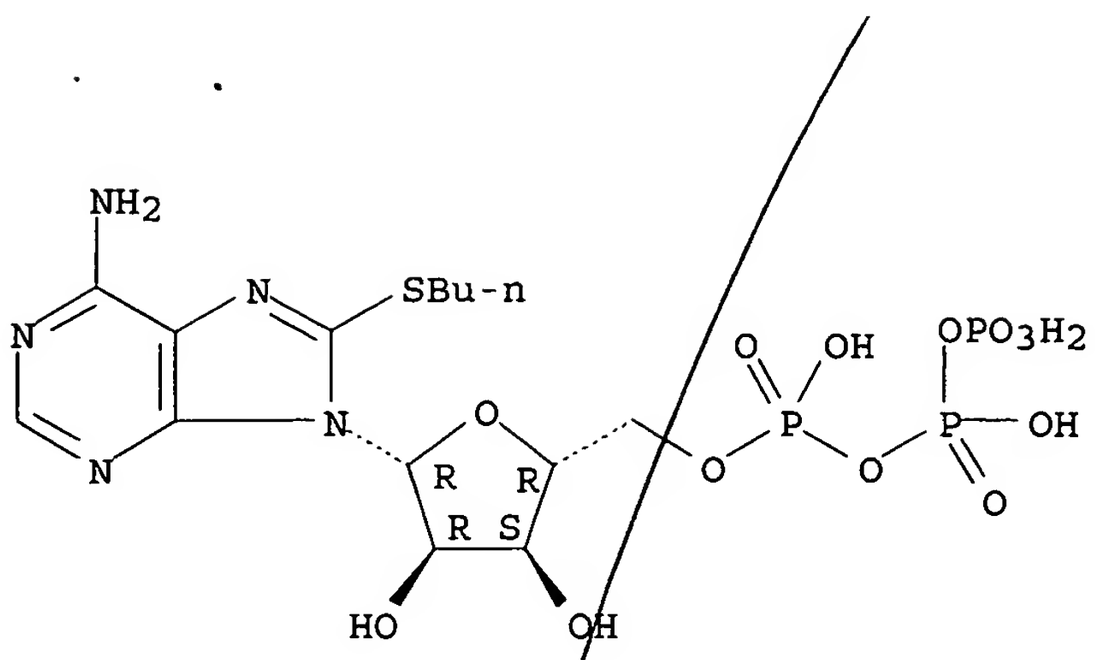
Absolute stereochemistry.



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

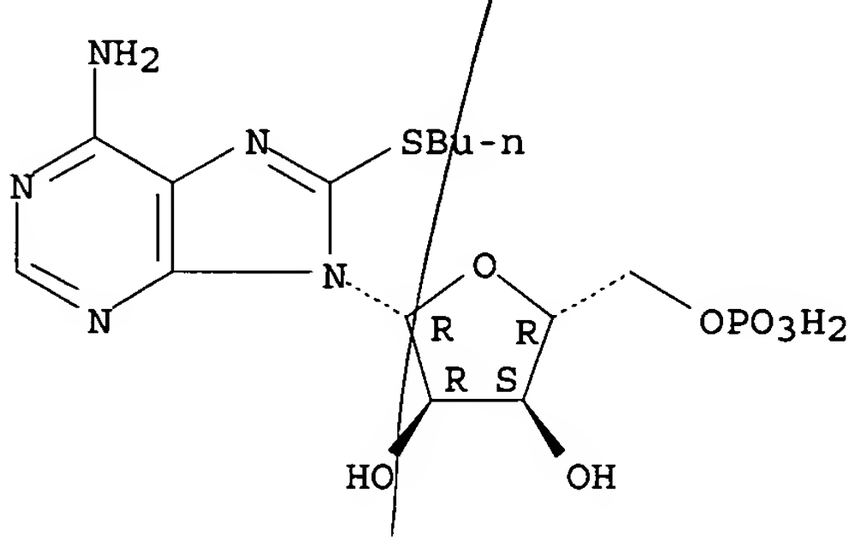
L8 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2001:293376 CAPLUS
DN 135:41096
TI Novel modified adenosine 5'-triphosphate analogues pharmacologically characterized in human embryonic kidney 293 cells highly expressing rat brain P2Y1 receptor: biotinylated analogue potentially suitable for specific P2Y1 receptor isolation
AU Zundorf, G.; Schafer, R.; Vohringer, C.; Halbfinger, E.; Fischer, B.; Reiser, G.
CS Medizinische Fakultat, Institut fur Neurobiochemie, Otto-von-Guericke-Universitat, Magdeburg, D-39120, Germany
SO Biochemical Pharmacology (2001), 61(10), 1259-1269
CODEN: BCPCA6; ISSN: 0006-2952
PB Elsevier Science Inc.
DT Journal
LA English
AB Rat brain P2Y1 (rP2Y1) receptor-transfected human embryonic kidney cells (HEK 293) were recently shown to have enhanced reactivity to both ATP and ADP. Here, the authors demonstrated the usefulness of this cell line as a system for further studying novel adenine nucleotide analogs and for the biochem. characterization of the P2Y1 receptor. By measurement of intracellular Ca2+ release, for 2-butylthio-, 2-butylamino-, and 2-butyloxy-ATP (2-BuS-, 2-BuNH-, 2-BuO-ATP), EC50 values of 1.3, 5, and 60 nM were determined, markedly lower than the value for ATP (130 nM). The EC50 for 2-BuSADP was 1.1 nM. The corresponding 8-substituted ATP analogs showed a substantially lower potency than ATP (ATP > 8-BuSATP > 8-BuNHATP ≈ 8-BuOATP). AMP induced intracellular Ca2+ release with a very low potency; 2- and 8-substitutions on AMP caused no significant potency shift, except for 2-BuSAMP (EC50 = 180 nM). Another new P2Y receptor probe, 2-[(6-biotinylamido)-hexylthio]ATP, was 22-fold more potent than ATP (EC50 = 6 nM), revealing that even more bulky substituents linked to the C-2 position bind with high affinity at the P2Y1 receptor. This biotinylated probe was successfully used for the enrichment of the P2Y1 receptor tagged with green fluorescent protein from a crude membrane fraction. This one-step enrichment provides a substantial advance for P2Y1 receptor purification Thus, human embryonic kidney 293 cells stably transfected with the rP2Y1 receptor represent a powerful model system for pharmacol. characterization of the P2Y1 receptor, circumventing problems associated with natural systems. They provide a means for the development of P2Y1 ligands of high potency and a good source for obtaining purified P2Y1 receptor.
IT **284040-54-6P 344402-39-7P**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(ATP analogs pharmacol. characterized in HEK293 cells expressing rat brain P2Y1 receptor in relation to biotinylated analog potentially suitable for specific P2Y1 receptor isolation)
RN 284040-54-6 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 344402-39-7 CAPLUS
CN 5'-Adenylic acid, 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2000:304989 CAPLUS
DN 133:105244
TI Novel Inhibitors of Nucleoside Triphosphate Diphosphohydrolases: Chemical Synthesis and Biochemical and Pharmacological Characterizations
AU Gendron, Fernand-Pierre; Halbfinger, Efrat; Fischer, Bilha; Duval, Martine; D'Orleans-Juste, Pedro; Beaudoin, Adrien R.
CS Department de Biologie, Universite de Sherbrooke, Sherbrooke, QC, J1K 2R1, Can.
SO Journal of Medicinal Chemistry (2000), 43(11), 2239-2247
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB To elucidate the physiol. role played by nucleoside triphosphate diphosphohydrolase (NTPDase; EC 3.6.1.5), adenine nucleotide analogs, modified on the purine ring, have been synthesized and tested as potential inhibitors. Resistance of ATP analogs to hydrolysis and their potency as NTPDase inhibitors were evaluated. For this purpose, a particulate fraction isolated from bovine spleen was used as the enzyme source. Among the synthesized analogs, 8-thiobutyladenosine 5'-triphosphate (8-BuS-ATP) was found to be the most effective nonhydrolyzable competitive inhibitor, with an estimated Ki of 10 μM. This nonhydrolyzable analog did not exert any P2X-receptor-mediated effect on endothelium-denuded blood vessels, from the guinea pig mesenteric bed. In agreement with this observation, infusion of the analog did not cause any significant blood pressure variations of the precontracted vessel. Because in previous studies on isolated turkey erythrocytes and rat astrocytes 8-BuS-ATP was not able to trigger any P2Y1-receptor-mediated effect, it therefore appears that this NTPDase inhibitor does not interfere with purinergic receptors.
IT **284040-53-5 284040-54-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(synthesis and biochem. and pharmacol. characterizations of novel

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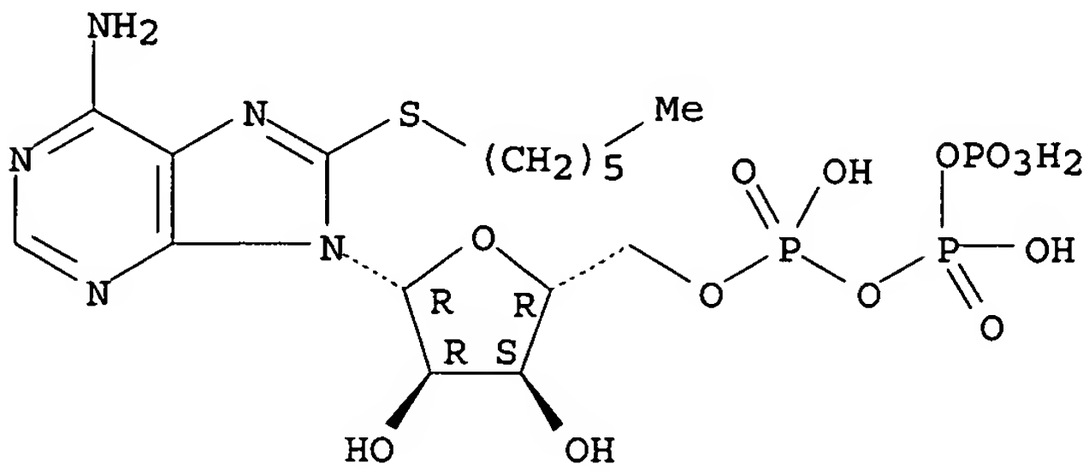
inhibitors of nucleoside triphosphate diphosphohydrolases)

RN 284040-53-5 CAPLUS

CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(hexylthio)- (9CI) (CA INDEX NAME)

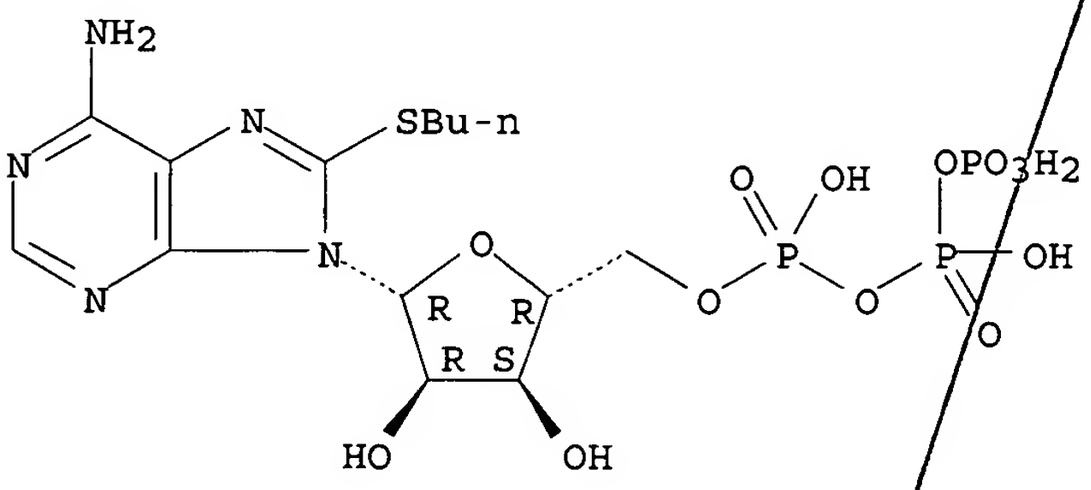
Absolute stereochemistry.



RN 284040-54-6 CAPLUS

CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **81609-35-0P 284040-51-3P 284040-52-4P**

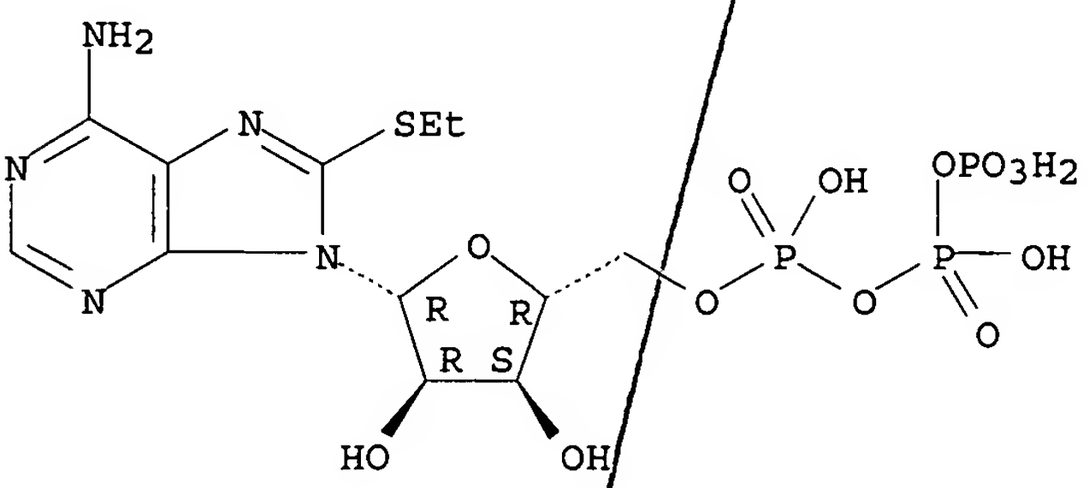
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and biochem. and pharmacol. characterizations of novel inhibitors of nucleoside triphosphate diphosphohydrolases)

RN 81609-35-0 CAPLUS

CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(ethylthio)- (9CI) (CA INDEX NAME)

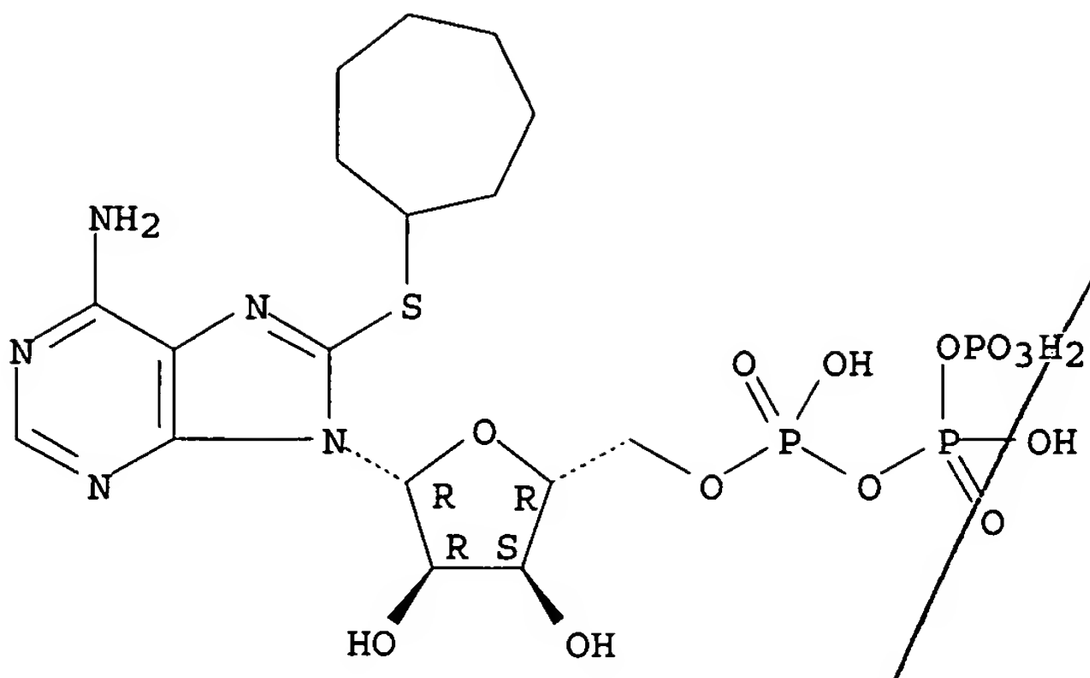
Absolute stereochemistry.



RN 284040-51-3 CAPLUS

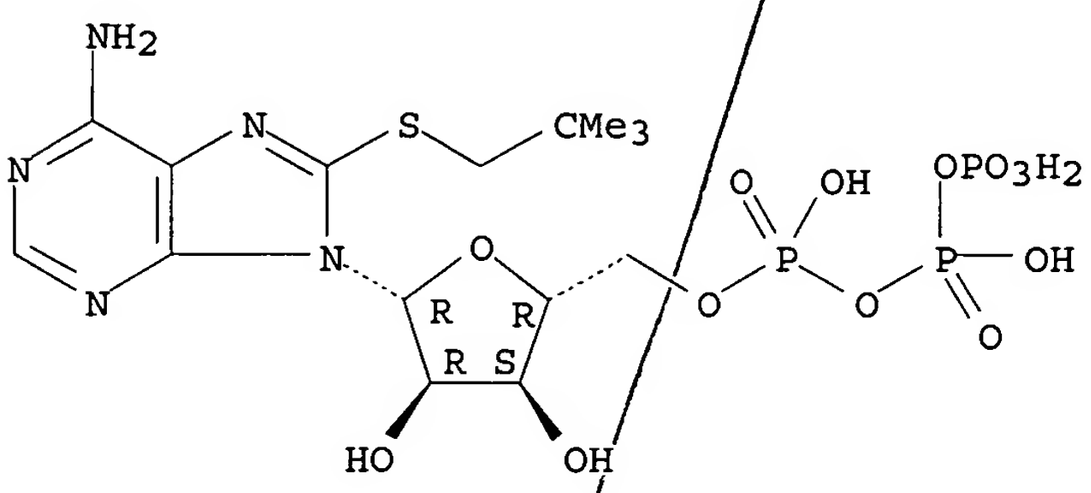
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(cycloheptylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 284040-52-4 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-[(2,2-dimethylpropyl)thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

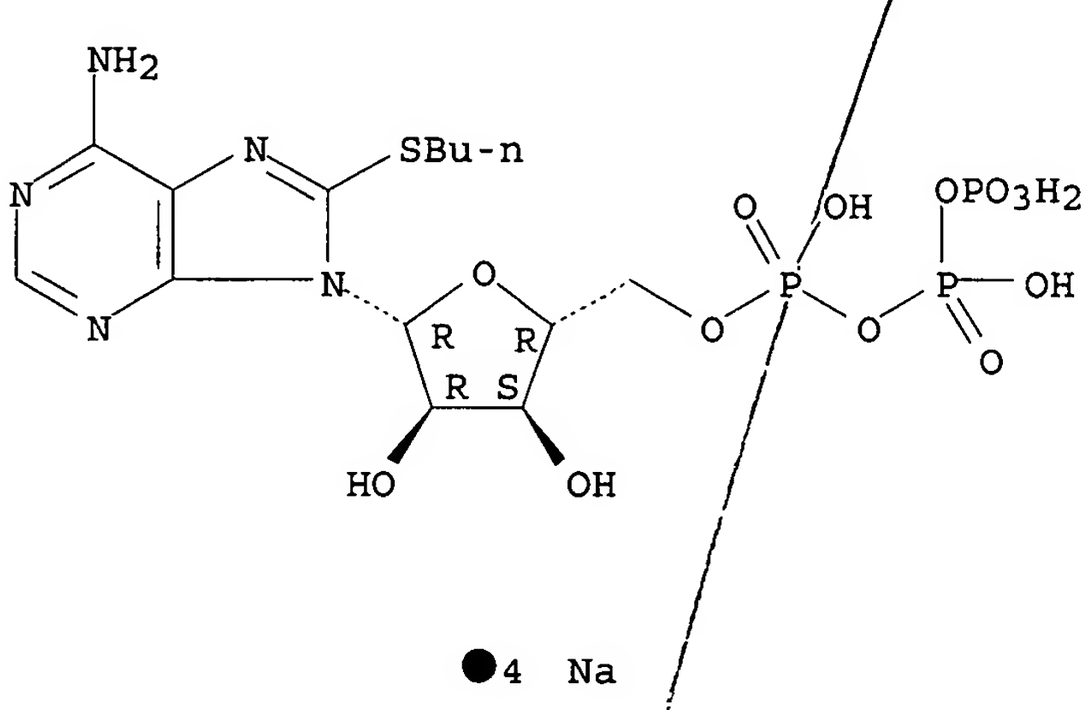
L8 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1999:771170 CAPLUS
DN 132:102410
TI Molecular Recognition of Modified Adenine Nucleotides by the P2Y1-Receptor. 1. A Synthetic, Biochemical, and NMR Approach
AU Halbfinger, Efrat; Major, Dan T.; Ritzmann, Marco; Ubl, Joachim; Reiser, Georg; Boyer, Jose L.; Harden, Kendall T.; Fischer, Bilha
CS Department of Chemistry Gonda-Goldschmied Center, Bar-Ilan University, Ramat-Gan, 52900, Israel
SO Journal of Medicinal Chemistry (1999), 42(26), 5325-5337
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB The remarkably high potencies of 2-thioether-adenine nucleotides regarding the activation of the P2Y1-receptor (P2Y1-R) in turkey erythrocyte membranes represent some of the largest substitution-promoted increases in potencies over that of a natural receptor ligand. This paper describes the investigation regarding the origin of the high potency of these P2Y1-R ligands over that of ATP. For this study, an integrated approach was employed combining the synthesis of new ATP analogs, their biochem. evaluation, and their SAR anal. involving NMR expts. and theor. calcns. These expts. and calcns. were performed to elucidate the conformation and to evaluate the electronic nature of the investigated P2Y1-R ligands. ATP analogs synthesized included derivs. where C2 or C8 positions were substituted with electron-donating groups such as ethers, thioethers, or amines. The compds. were tested for their potency to induce P2Y1-R-mediated activation of phospholipase C in turkey erythrocytes and Ca2+ response in rat astrocytes. 8-Substituted ATP and AMP derivs. had

little or no effect on phospholipase C or on calcium levels, whereas the corresponding 2-substituted ATP analogs potently increased the levels of inositol phosphates and [Ca2+]i. AMP analogs were ineffective except for 2-butylthio-AMP which induced a small Ca2+ response. P2Y1-R activity of these compds. was demonstrated by testing these ligands also on NG108-15 neuroblastoma + glioma hybrid cells. NMR data together with theor. calcns. imply that steric, rather than electronic, effects play a major role in ligand binding to the P2Y1-R. Hydrophobic interactions and H-bonds of the C2 substituent appear to be important determinants of a P2Y1-R ligand affinity.

IT **71683-16-4P 255716-10-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and structure activity relations of modified adenine nucleotides as P2Y1 receptor agonists)

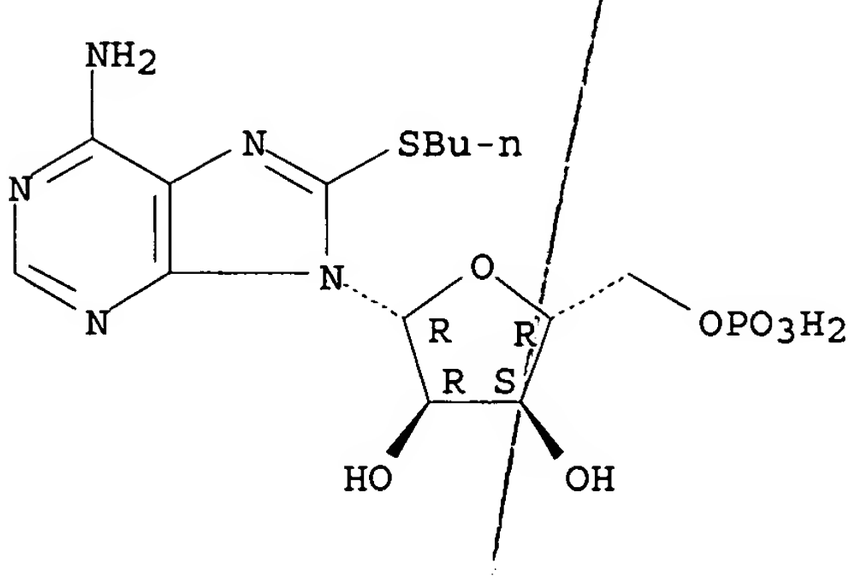
RN 71683-16-4 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)-, tetrasodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 255716-10-0 CAPLUS
CN 5'-Adenylic acid, 8-(butylthio)-, disodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1997:804940 CAPLUS
DN 128:164073
TI Quantitative one step derivatization of oligonucleotides by a fluorescent label through abasic site formation

AU Boturyn, Didier; Defrancq, Eric; Ducros, Veronique; Fontaine, Catherine; Lhomme, Jean

CS LEDSS, UMR 5616, Universite Joseph Fourier - Grenoble I, GRENOBLE, 38041, Fr.

SO Nucleosides & Nucleotides (1997), 16(10 & 11), 2069-2077
CODEN: NUNUD5; ISSN: 0732-8311
PB Marcel Dekker, Inc.
DT Journal
LA English

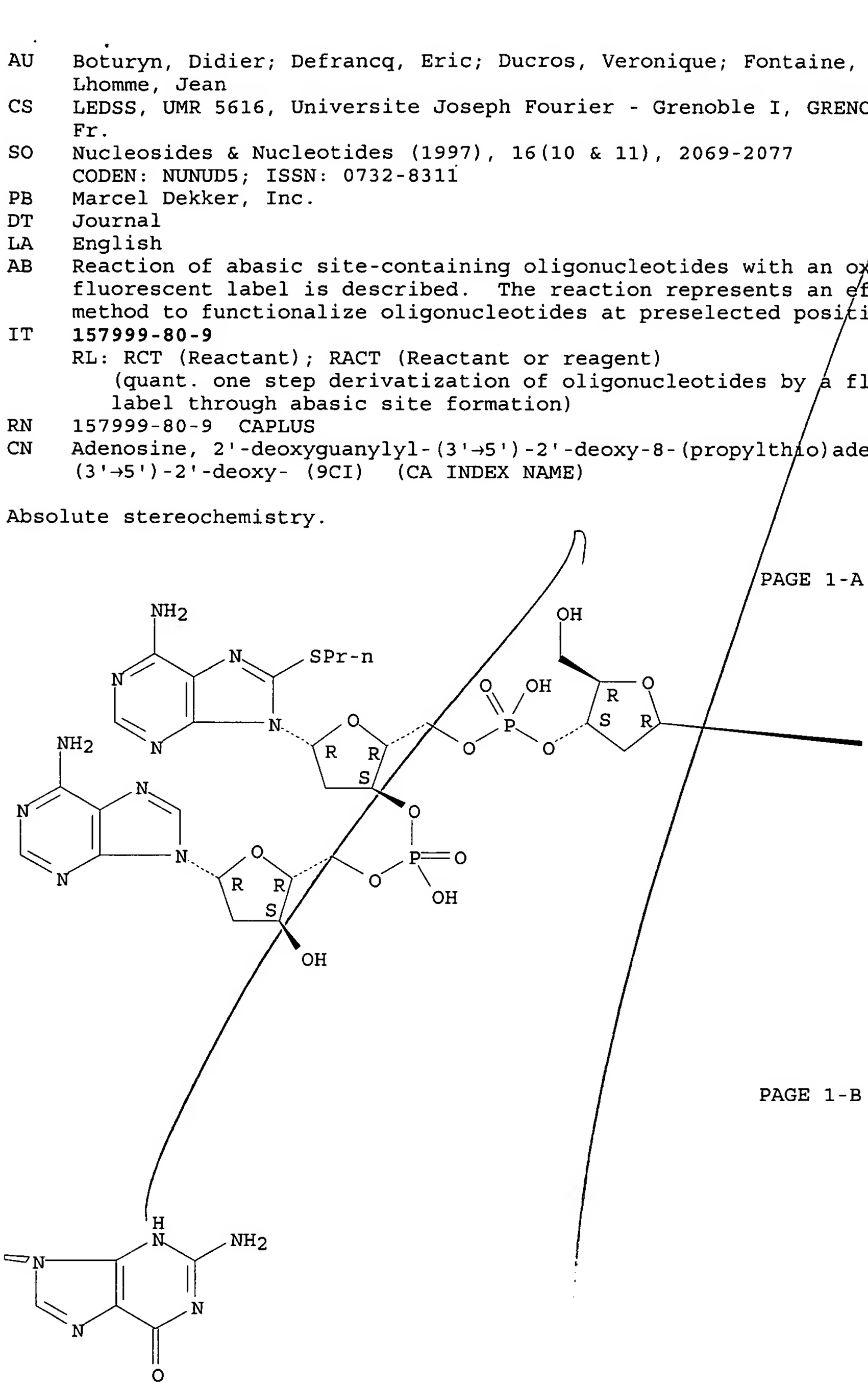
AB Reaction of abasic site-containing oligonucleotides with an oxyamino fluorescent label is described. The reaction represents an efficient method to functionalize oligonucleotides at preselected positions.

IT **157999-80-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(quant. one step derivatization of oligonucleotides by a fluorescent label through abasic site formation)

RN 157999-80-9 CAPLUS

CN Adenosine, 2'-deoxyguanylyl-(3'→5')-2'-deoxy-8-(propylthio)adenylyl-(3'→5')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



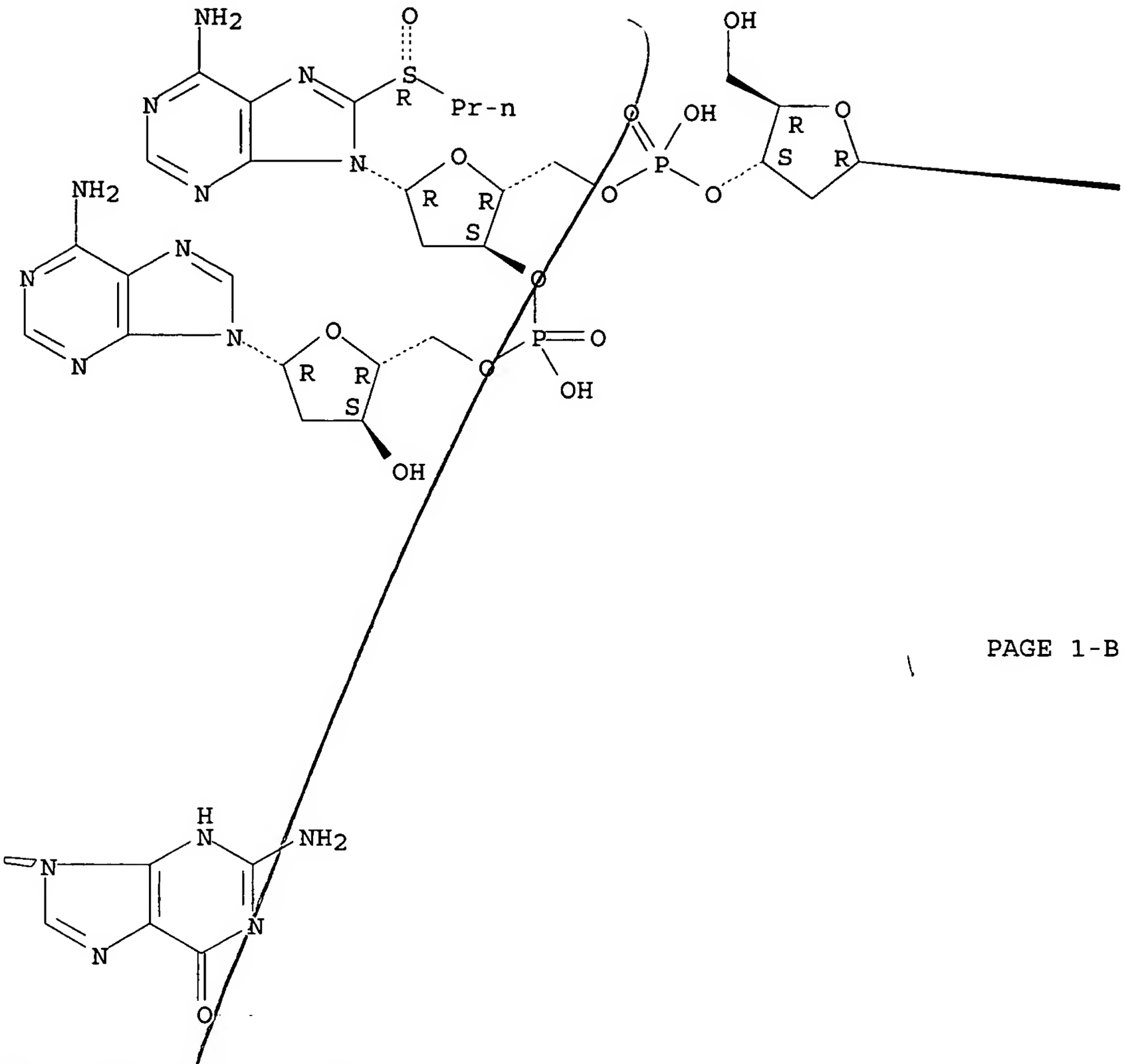
IT **202598-24-1P 202598-26-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(quant. one step derivatization of oligonucleotides by a fluorescent label through abasic site formation)

RN 202598-24-1 CAPLUS

CN Adenosine, 2'-deoxyguanylyl-(3'→5')-2'-deoxy-8-[(R)-propylsulfinyl]adenylyl-(3'→5')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

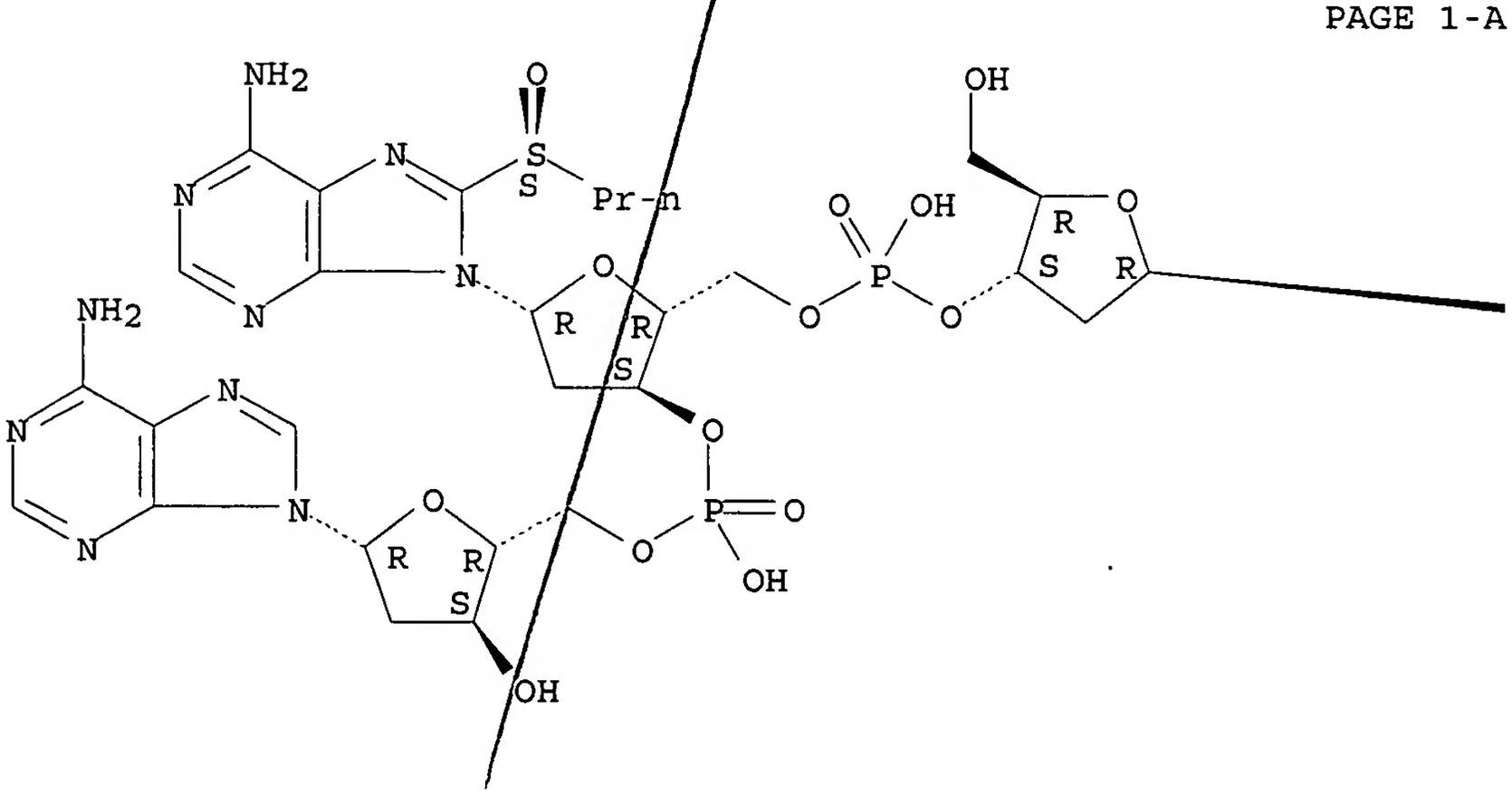


PAGE 1-B

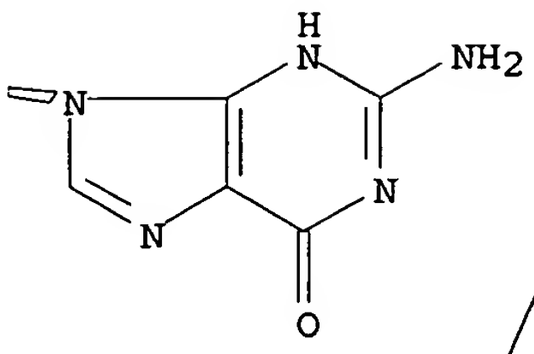
RN 202598-26-3 CAPLUS
CN Adenosine, 2'-deoxyguanylyl-(3'→5')-2'-deoxy-8-[(S)-propylsulfinyl]adenylyl-(3'→5')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

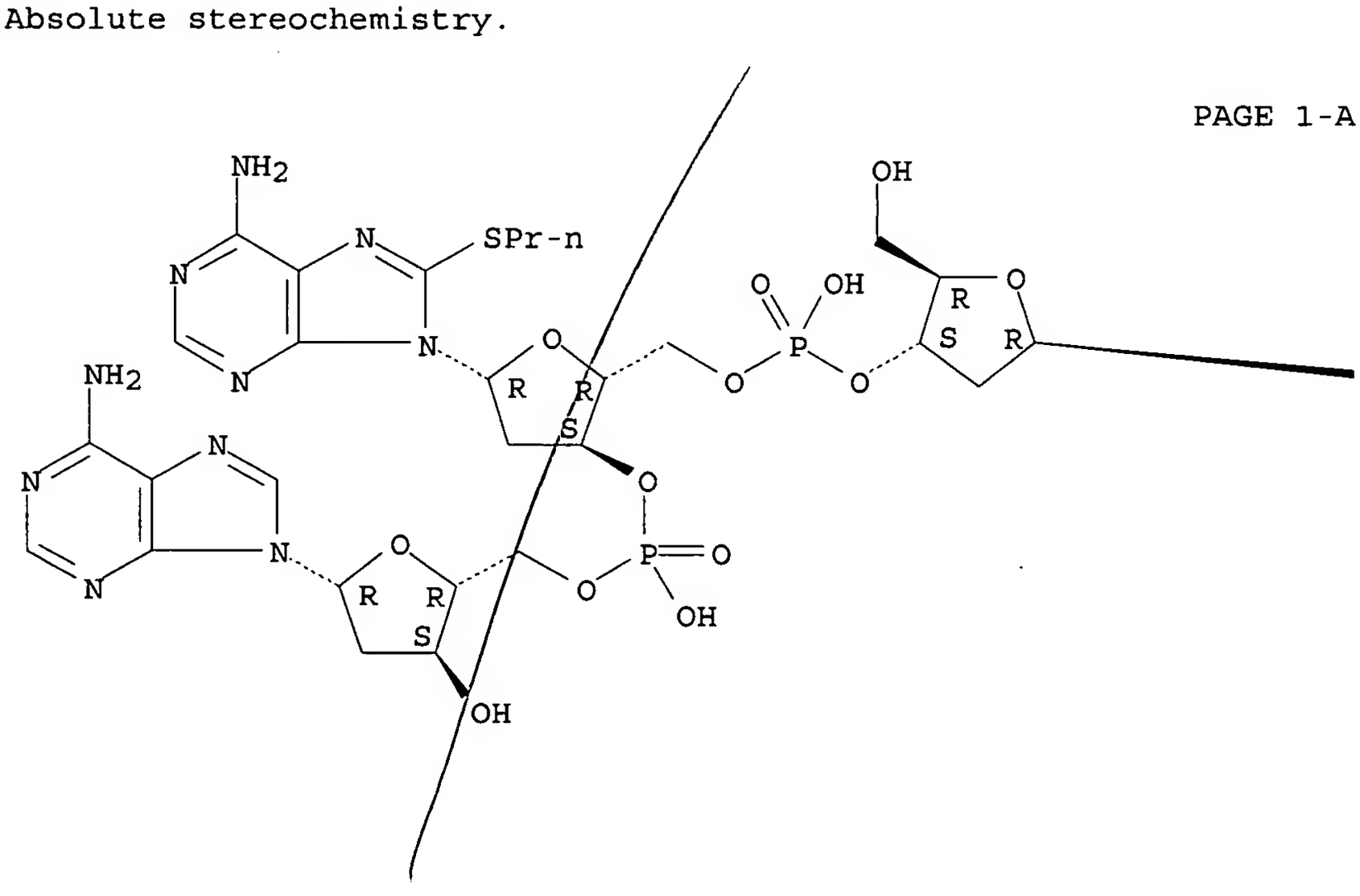


RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

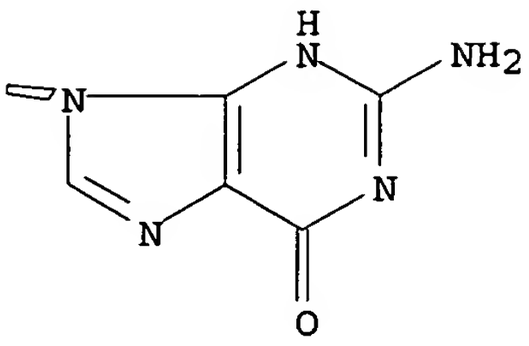
L8 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1994:605872 CAPLUS
DN 121:205872
TI Hydrolysis of oligodeoxyribonucleotides containing 8-substituted purine nucleosides. A new route for preparing abasic oligodeoxyribonucleotides
AU Laayoun, Ali; Decout, Jean-Luc; Defrancq, Eric; Lhomme, Jean
CS L.E.D.S.S., URA CNRS, Univ. Joseph Fourier, Grenoble, 38041, Fr.
SO Tetrahedron Letters (1994), 35(28), 4991-4
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
AB 2'-Deoxyadenosine substituted at C-8 by a propylthio group was introduced into oligodeoxyribonucleotides by solid phase synthesis. Oxidation by potassium persulfate occurred selectively on the sulfur containing nucleoside causing a weakening of the glycosidic bond. Subsequent hydrolytic treatment led to selective removal of the modified base and generation of an abasic site. This constitutes a novel and convenient route for the chemical synthesis of oligodeoxyribonucleotides containing an abasic site at a preselected position in the sequence.
IT **157999-80-9P 158020-58-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)
RN 157999-80-9 CAPLUS
CN Adenosine, 2'-deoxyguanylyl-(3'→5')-2'-deoxy-8-(propylthio)adenylyl-(3'→5')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



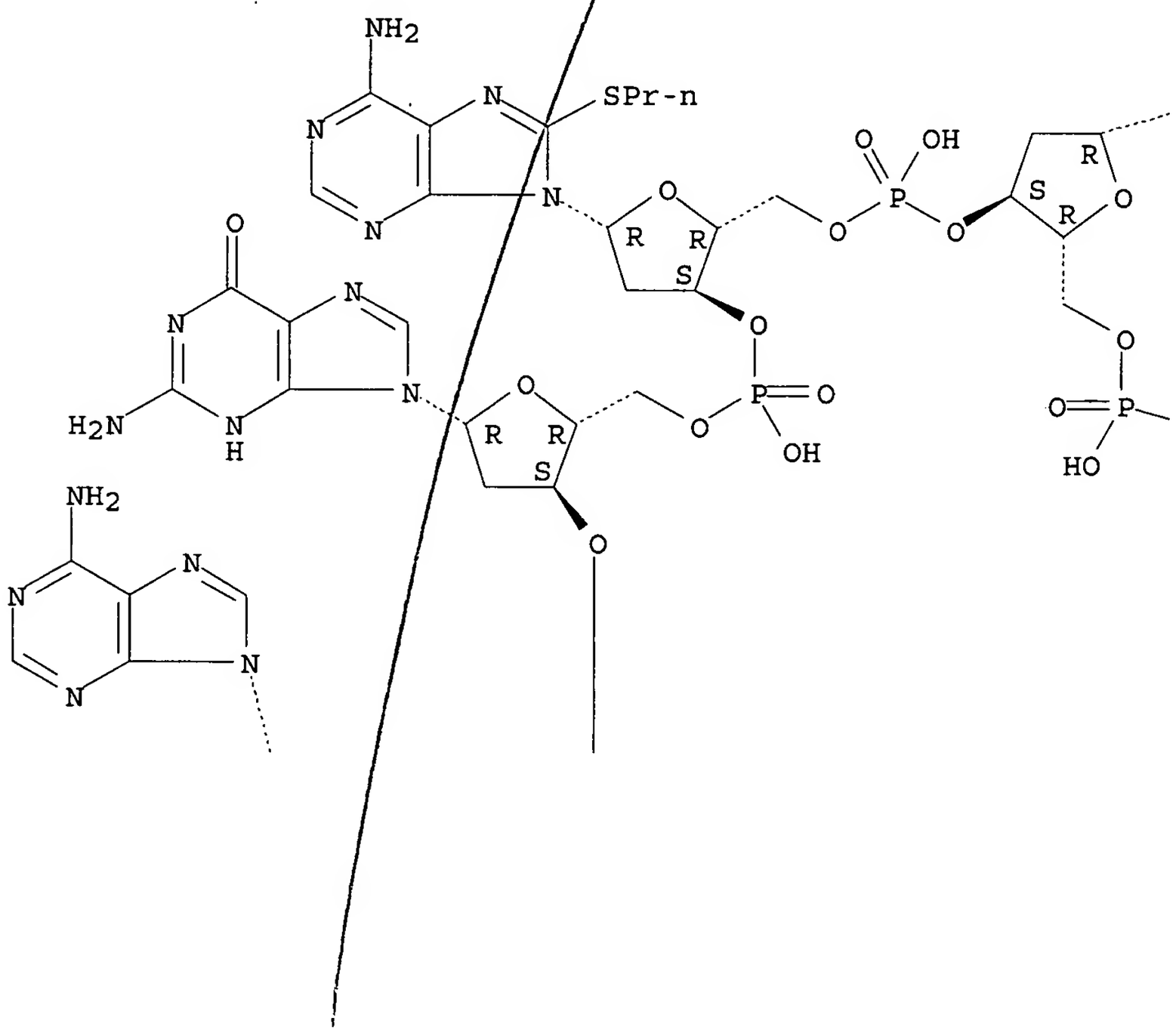
PAGE 1-B

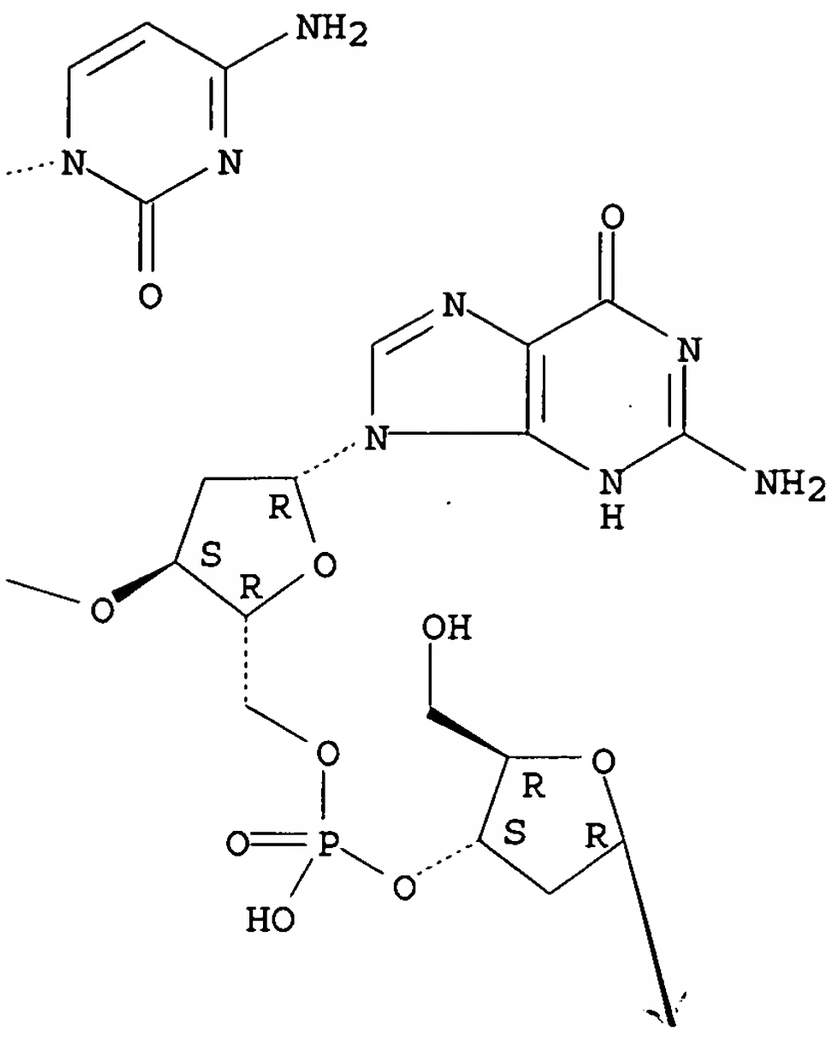


RN 158020-58-7 CAPLUS
CN Thymidine, 2'-deoxyadenylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxy-8-(propylthio)adenylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')- (9CI) (CA INDEX NAME)

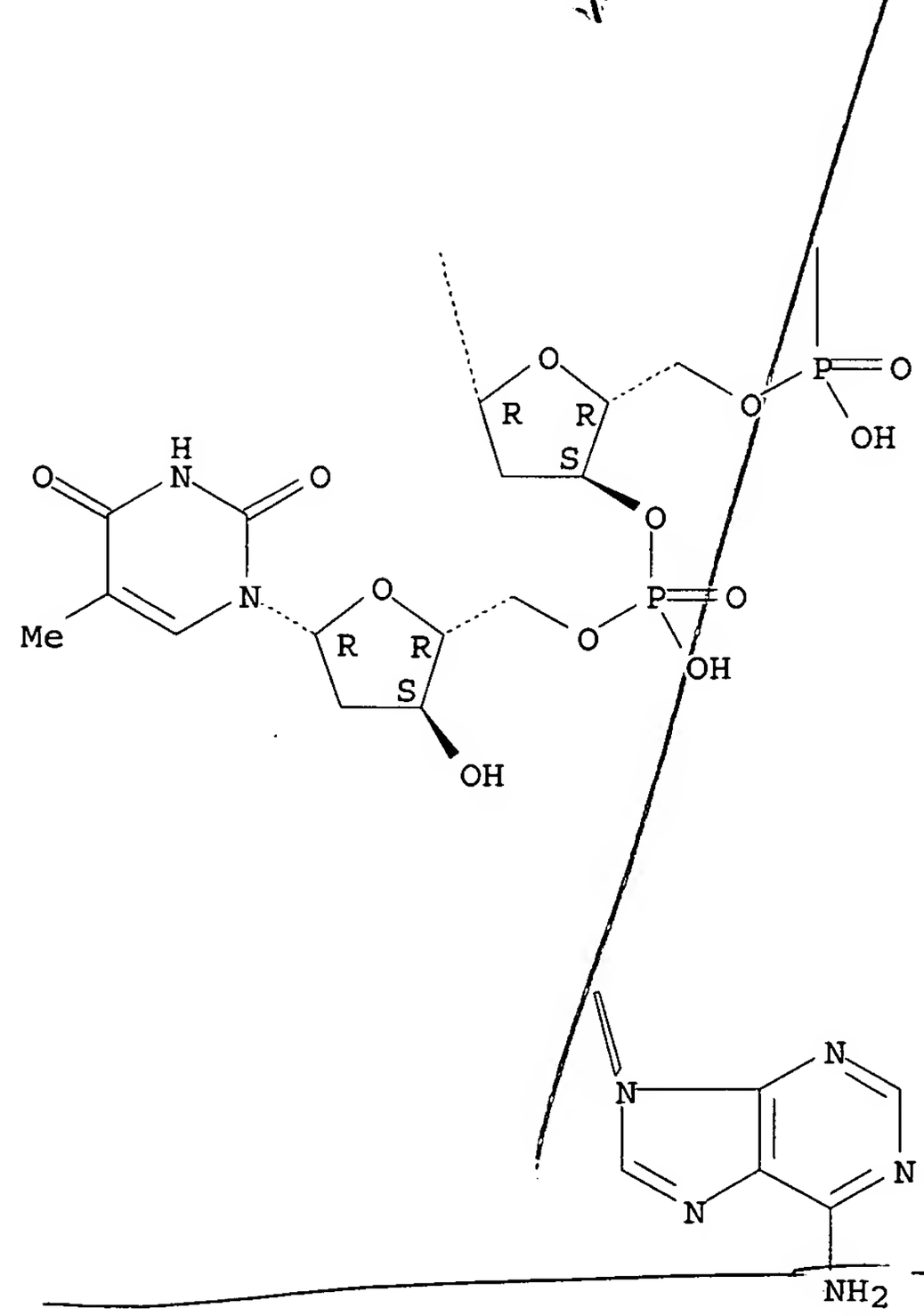
Absolute stereochemistry.

PAGE 1-A





PAGE 1-B



PAGE 2-A

PAGE 2-B

L8 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1982:616611 CAPLUS
DN 97:216611
TI Species- or isozyme-selective enzyme inhibitors. 8. Synthesis of disubstituted two-substrate condensation products as inhibitors of rat adenylate kinases
AU Kappler, Francis; Hai, Ton T.; Abo, Masanobu; Hampton, Alexander
CS Inst. Cancer Res., Fox Chase Cancer Cent., Philadelphia, PA, 19111, USA
SO Journal of Medicinal Chemistry (1982), 25(10), 1179-84

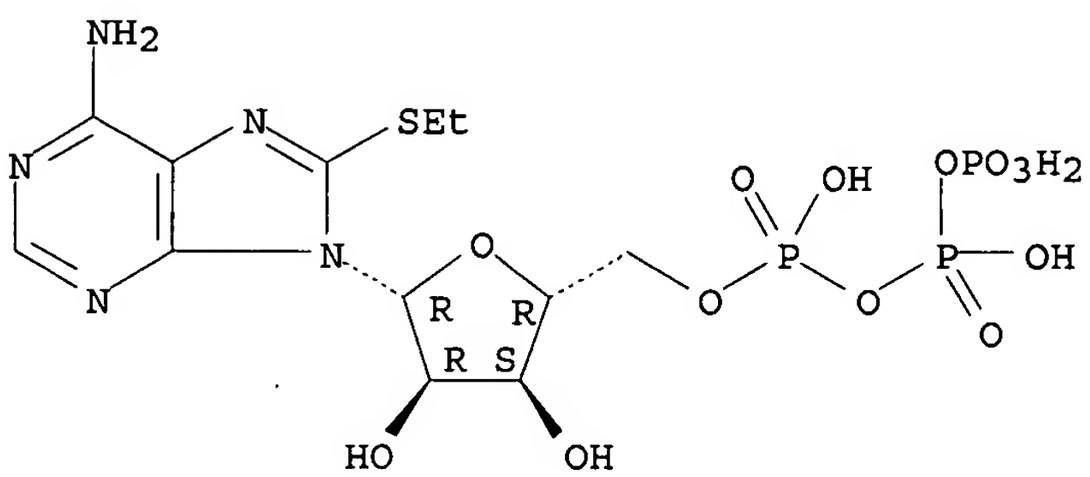
reads on parent case

CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
AB Syntheses are described of 5'(R)- and 5'(S)-C-Me-ATP, 5'(R)- and 5'(S)-C-n-Pr-ATP, and the phosphonate isostere of ATP with a C(5')-CH2-P system. Two of the five compds. inhibited rat muscle adenylate kinase (AK-M) 8-9.5 times more effectively than AK II (present in poorly differentiated rat hepatoma tissue) and the two other compds. inhibited AK II at least 2-fold more effectively than AK-M. P1-[8-Ethylthio adenosine-5']-P5-(adenosine-5') pentaphosphate (8-SEt-Ap5A) is a potent dual substrate site inhibitor of the rat isozymes with selectivity for AK II. Three derivs. of 8-SEt-Ap5A were synthesized: p1-[8-(ethylthio) adenosine-5')-p5-[5'(R)-C-methyladenosine-5'] pentaphosphate (I), its 5'(R)-C-n-Pr analog (II), and di(8-SEt)-Ap5A (III). I and II, are readily accessible via reaction of a derivative of ATP γ-piperidinate with an ADP derivative Except in the interaction of III with AK-M, I-III acted as two-site competitive inhibitors of AK-M and AK II. Inhibitory potencies of I-III with the two isozymes varied over more than a 95-fold range, and inhibitory potencies for AK-M relative to those of AK II varied more than 61-fold. III was an effective inhibitor of AK II and exhibited at least 4 times more selectivity for AK II than 8-SEt-Ap5A.
IT **83683-78-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with ADP derivative)
RN 83683-78-7 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(ethylthio)-, compd. with N,N-dibutyl-1-butanamine (1:4) (9CI) (CA INDEX NAME)

CM 1

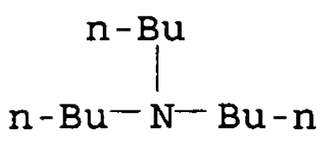
CRN 81609-35-0
CMF C12 H20 N5 O13 P3 S

Absolute stereochemistry.



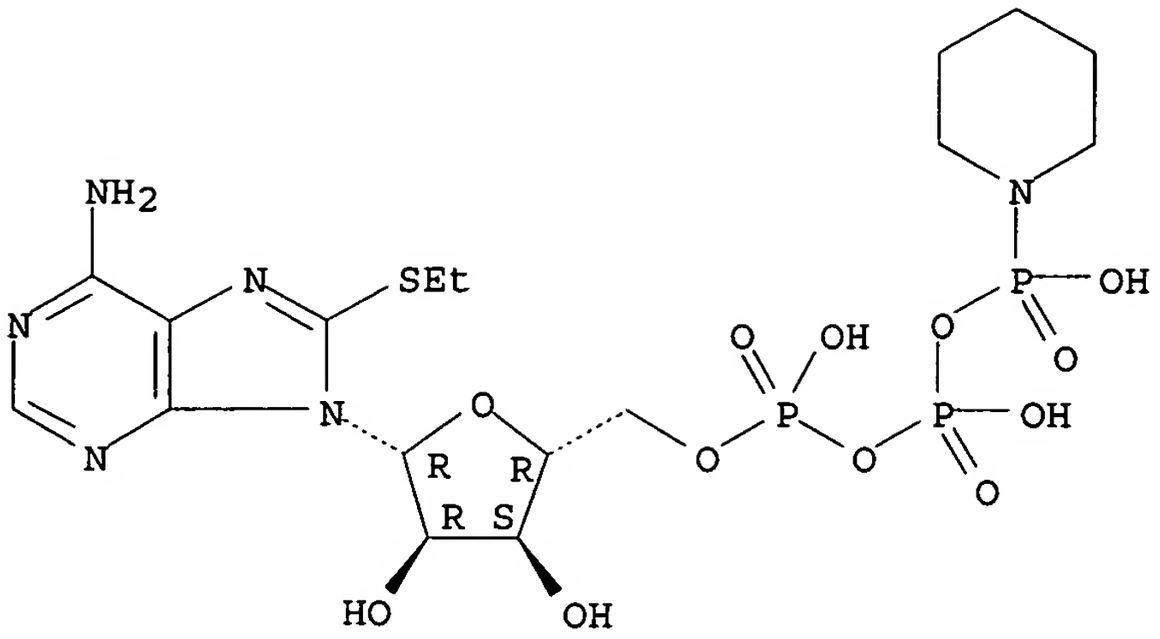
CM 2

CRN 102-82-9
CMF C12 H27 N



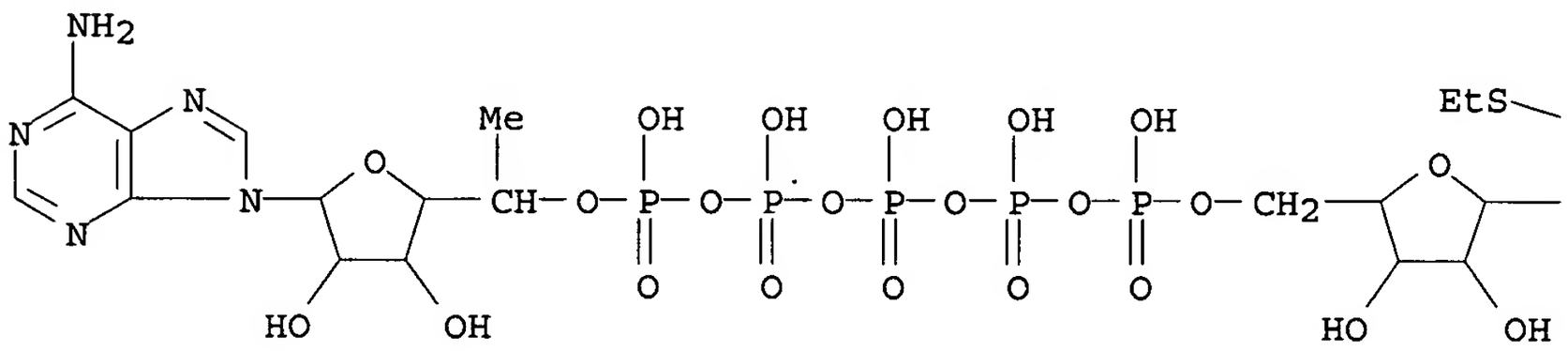
IT **83683-81-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and condensation reaction of, with ADP derivative)
RN 83683-81-2 CAPLUS
CN Adenosine 5'-(trihydrogen diphosphate), 8-(ethylthio)-, P'-anhydride with 1-piperidinylphosphonic acid (9CI) (CA INDEX NAME)

Absolute stereochemistry.



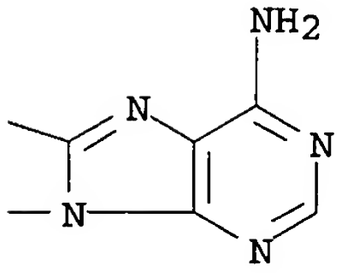
IT **83683-76-5P 83683-77-6P 83694-37-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and inhibition of adenylate kinases by)
RN 83683-76-5 CAPLUS
CN Adenosine 5'-(hexahydrogen pentaphosphate), 8-(ethylthio)-,
P''''→5'-ester with 9-(6-deoxy-β-D-allofuranosyl)-9H-purin-6-
amine, pentasodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



●5 Na

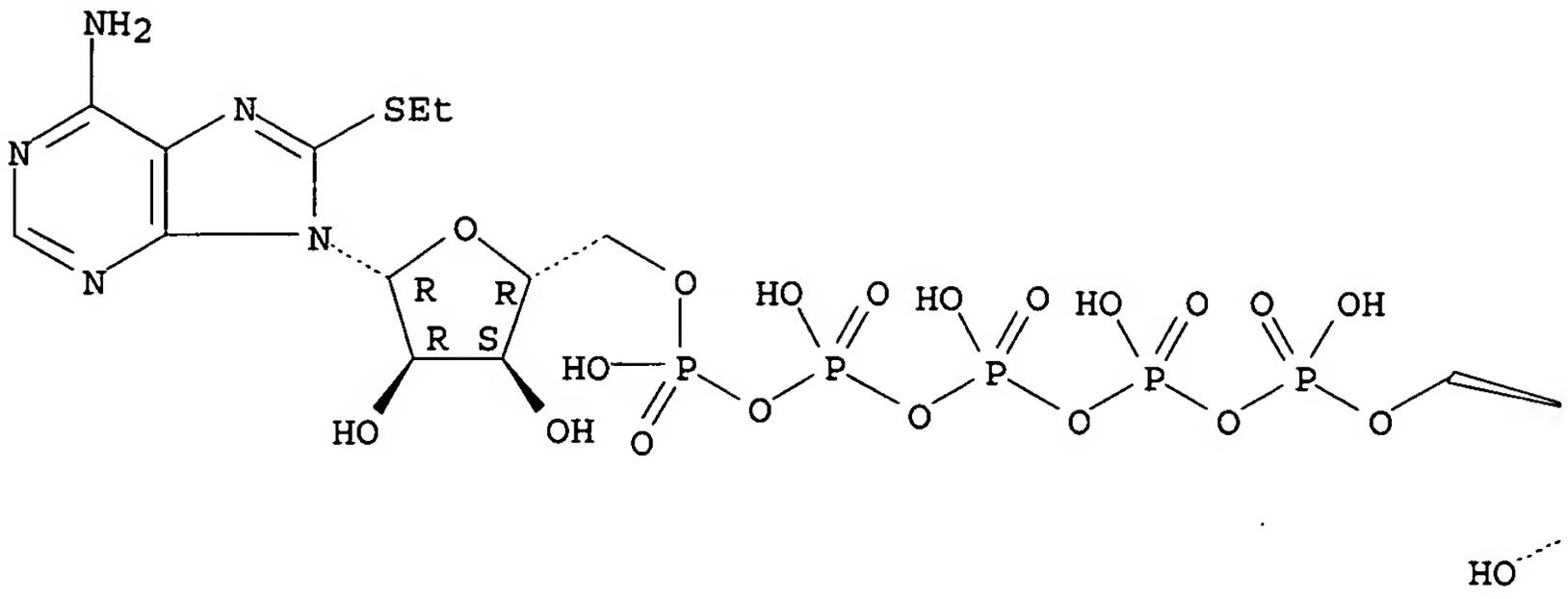
PAGE 1-B



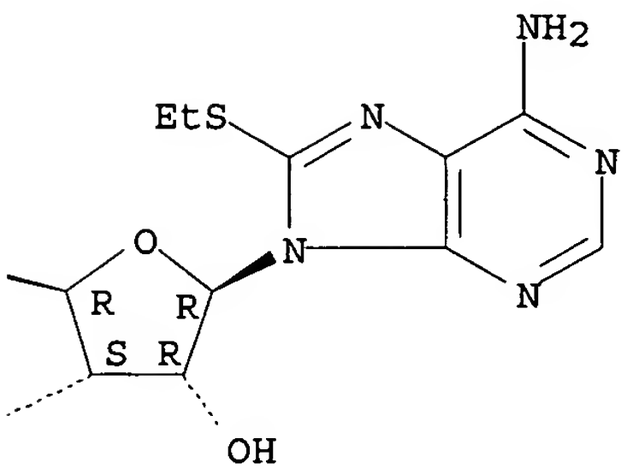
RN 83683-77-6 CAPLUS
CN Adenosine 5'-(hexahydrogen pentaphosphate), 8-(ethylthio)-,
P''''→5' ester with 8-(ethylthio)adenosine (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

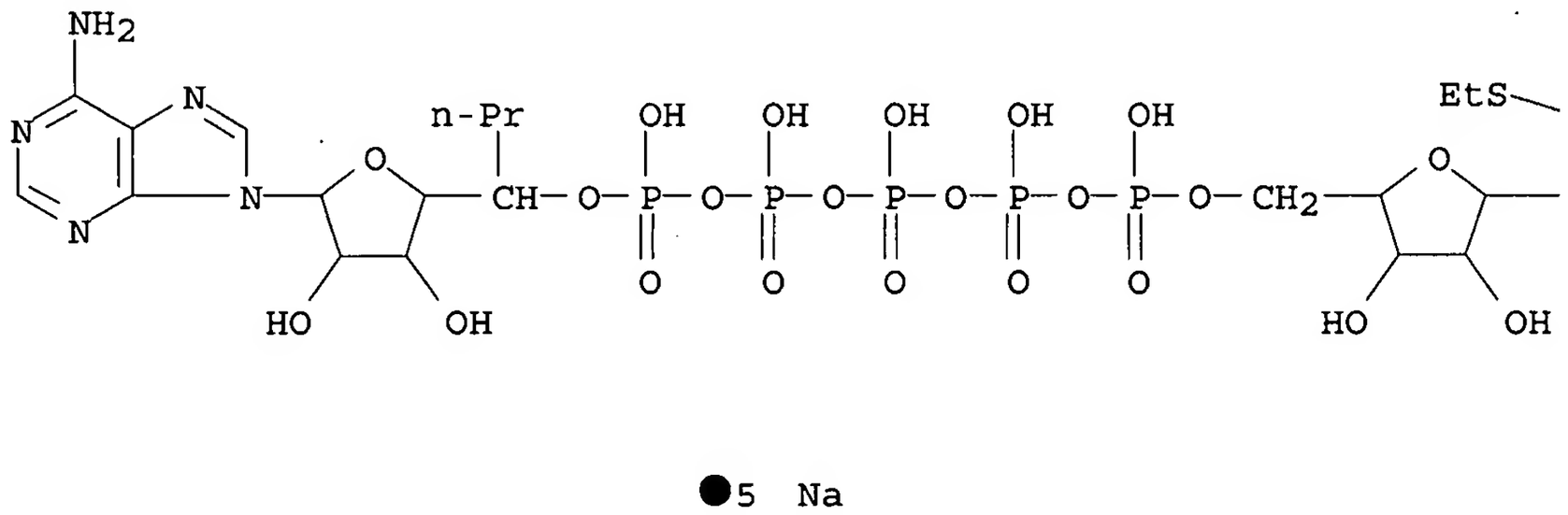


PAGE 1-B



RN 83694-37-5 CAPLUS
CN Adenosine 5'-(hexahydrogen pentaphosphate), 8-(ethylthio)-, P''''→5'-ester with 9-(6,7,8-trideoxy-β-D-allo-octofuranosyl)-9H-purin-6-amine, pentasodium salt (9CI) (CA INDEX NAME)

PAGE 1-A

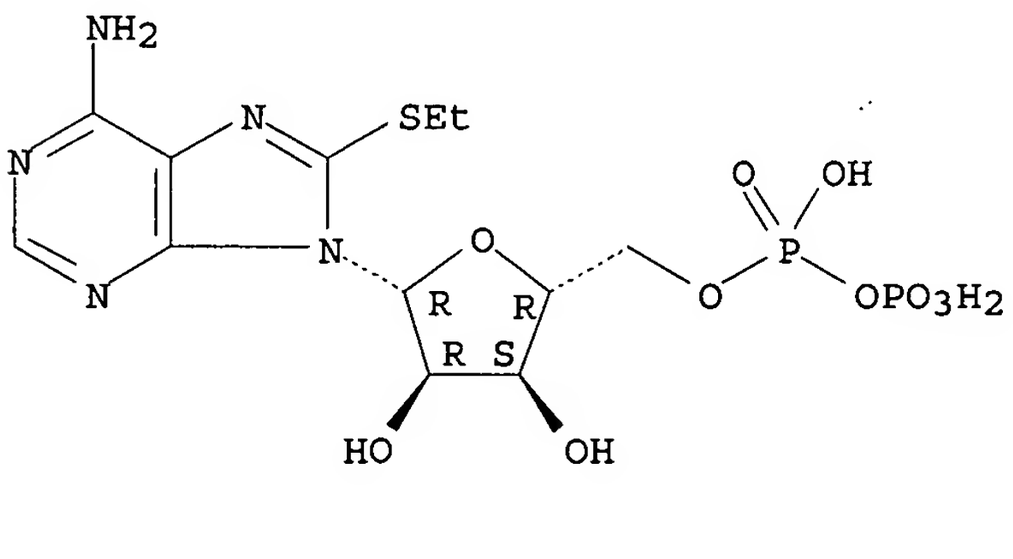


●5 Na

PAGE 1-B

L8 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1982:611265 CAPLUS
DN 97:211265
TI Species- or isozyme-specific enzyme inhibitors. 9. Selective effects in inhibitions of rat pyruvate kinase isozymes by adenosine 5'-diphosphate derivatives
AU Hai, Ton T.; Abo, Masanobu; Hampton, Alexander
CS Fox Chase Cancer Cent., Inst. Cancer Res., Philadelphia, PA, 19111, USA
SO Journal of Medicinal Chemistry (1982), 25(10), 1184-8
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
AB Derivs. of ADP with a substituent of 1-4 atoms at any of 8 positions were synthesized and evaluated as substrates and inhibitors of the liver (L), muscle (M), and kidney (K) isoenzymes of rat pyruvate kinase (I). The inhibitory potencies of the compds. were expressed as Km (ADP)/Ki or as Km (ADP)/Km when no Ki value was available. Nine of 14 ADP derivs. exhibited differential inhibitions. The M and K isoenzymes, which cross-react immunol. with each other, but not with the L form, were inhibited differentially by 5 of the 14 derivs. I-K was preferentially inhibited by 2 derivs., I-L by 3 derivs., and I-M by 2 derivs. Among the most selective and/or effective inhibitors were 3'-OMe-ADP [Km (ADP)/Ki = 0.07 with I-K; inhibitory potency, K:M:L, 7.6:6.0:1], N6-Me,N6-(CH2)4N(Me)COMe-ADP (prepared previously) [Km (ADP)/Km = 0.43 with I-L; inhibitory potency, L:K:M, 3:2:1], and 8-NHEt-ADP [Km (ADP)/Ki = 1.0 with I-M; inhibitory potency, M:K:L, 7.1:1.2:1]. These and previous studies with 2 other enzymes indicate that monosubstituted substrate derivs. that bear short substituents (usually 1-4 atoms) at various positions are potentially useful probes in early stages of the attempted design of isoenzyme-selective inhibitors.
IT **81609-45-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reaction kinetics with pyruvate kinase isoenzymes)
RN 81609-45-2 CAPLUS
CN Adenosine 5'-(trihydrogen diphosphate), 8-(ethylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1982:402705 CAPLUS
DN 97:2705
TI Species- or isozyme-specific enzyme inhibitors. 7. Selective effects in inhibitions of rat adenylate kinase isozymes by adenosine 5'-phosphate derivatives
AU Hai, Ton T.; Picker, Donald; Abo, Masanobu; Hampton, Alexander
CS Fox Chase Cancer Cent., Inst. Cancer Res., Philadelphia, PA, 19111, USA
SO Journal of Medicinal Chemistry (1982), 25(7), 806-12
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
AB Monosubstituted derivs. of AMP with substituents of 1-3 atoms or group replacements at any of 11 positions were synthesized and examined as substrates and inhibitors of the rat muscle adenylate kinase isoenzyme

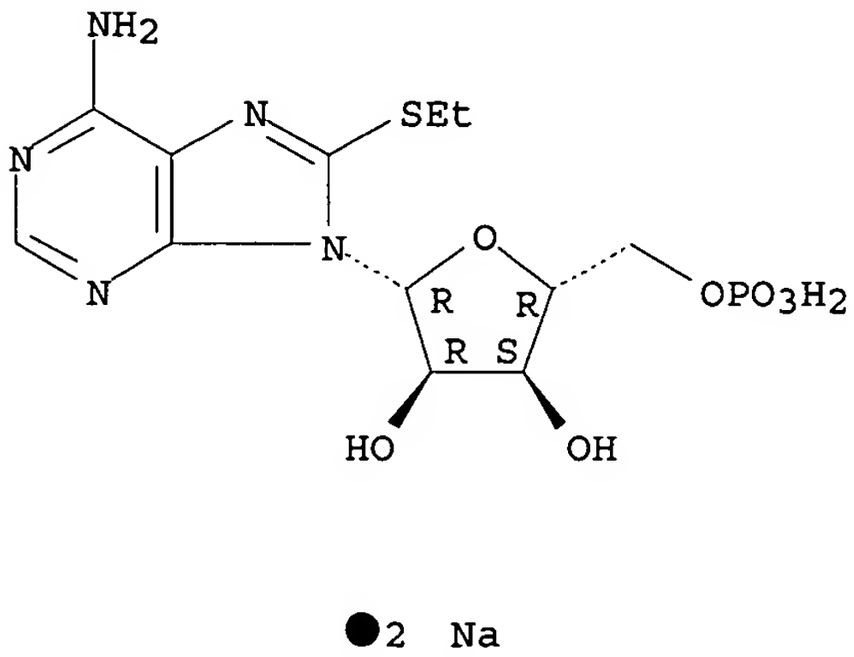
(AK-M) and the rat AK II and III isoenzymes predominant in poorly differentiated hepatoma tissue and normal liver tissue, resp. Inhibition indexes of the compds. were expressed as Km(AMP)/Ki for competitive inhibition or as Km(AMP)/Km when only Km was available. Substituents at N(1), N6, or C(8) or on the ionizable phosphate O atom reduced inhibition below measurable levels; 2'-deoxy-AMP and adenosine 5'-sulfate had identical inhibition indexes with all 3 isoenzymes; compds. with substituents at C(2), O(2'), O(3'), C(4'), C(5'), or O(5') had higher inhibition indexes with AK-M than with AK II or III, and the same or similar indexes for AK II and III. The most effective and(or) selective inhibitors were 2-NHMe-AMP (index with AK-M, 0.2; index ratio, AK-M/AK III, 9.1), 2'-O-Me-AMP (index with AK-M, 0.14; index ratio, AK-M/AK III, 8.2), 2',3'-O-CMe2-AMP (index with AK-M, 0.25; index ratio, AK-M/AK II, 6.6), 4'-allyl-AMP (index with AK-M, 0.97; index ratio, AK-M/AK III, 8.1), and 5'(S)-Et-AMP (index with AK-M, 0.64; index ratio, AK-M/AK II, 11.2). The study provided addnl. evidence that the attachment of simple substituents to various atoms in turn of a substrate is a potentially useful approach in early stages of the attempted design of isoenzyme-selective inhibitors.

IT **81921-37-1**
RL: BIOL (Biological study)
(adenylate kinase isoenzyme inhibition by, structure in relation to)

RN 81921-37-1 CAPLUS

CN 5'-Adenylic acid, 8-(ethylthio)-, disodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1982:402685 CAPLUS
DN 97:2685
TI Species- or isozyme-specific enzyme inhibitors. 4. Design of a two-site inhibitor of adenylate kinase with isozyme selectivity
AU Hampton, Alexander; Kappler, Francis; Picker, Donald
CS Inst. Cancer Res., Fox Chase Cancer Cent., Philadelphia, PA, 19111, USA
SO Journal of Medicinal Chemistry (1982), 25(6), 638-44
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
AB The ATP analogs, 6-butylamino-, 6-dibutylamino-, and 6-butylthio-9β-D-ribofuranosylpurine 5'-triphosphate (I, II, and III, resp.), were synthesized and studied as inhibitors and(or) substrates of the rat muscle adenylate kinase isoenzyme (AK M) and the rat liver isoenzymes AK II and III. I and III were substrates (Vmax relative to ATP, 13-190%) of the 3 AK isoenzymes, whereas II was a weak substrate and a competitive inhibitor of AK M and AK III. The affinities of the analogs relative to ATP [Km (ATP)/Km or Ki] were 0.03-0.075 for AK III and 0.14-0.28 for AK M, and the affinities for AK M exceeded those for AK III by factors of 2.3-7.0. Ap5A was synthesized by an improved method and was found to be a potent 2-site inhibitor (Ki = 0.28 μM), competitive toward AMP or ATP, for the 3 AK isoenzymes. 8-Ethylthio-Ap5A (IV) also behaved as a 2-site inhibitor; the 8-ethylthio group reduced the affinity for AK M 12-fold, but increased the

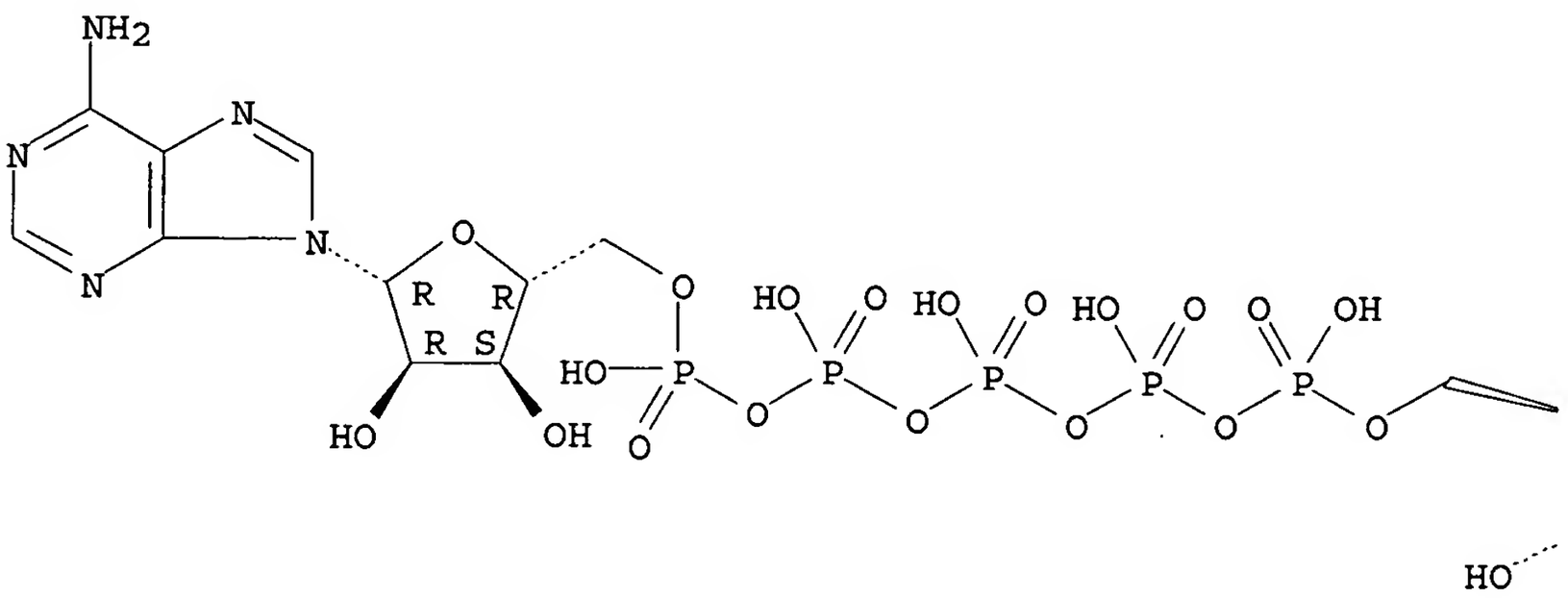
affinity for AK II and III 4-fold, resulting in .apprx.45-fold more effective inhibition of AK II and III (Ki = 0.07 μM) than of AK M (Ki = 3.25 μM). The 8-ethylthio group of 8-ethylthio-ATP (V) likewise reduced the affinity for the ATP site of AK M, but enhanced the affinity for the ATP sites of AK II and III, resulting in ≥30-fold more effective inhibition of AK II and III. 8-Ethylthio-AMP inhibited AK II and III noncompetitively (Ki = 21-24 mM) with respect to AMP, indicating that the 8-ethylthioadenosine moiety of IV probably binds to the ATP sites of these isoenzymes. IV had .apprx.1000-fold more affinity for AK II or III than did V. The findings indicate that isoenzyme-selective inhibitory effects of a substrate derivative can be imparted to a 2-site inhibitor, leading to significant enhancement of inhibitory potency.

IT **81609-34-9P 81609-35-0P 81609-36-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and adenylate kinase isoenzyme inhibition by)

RN 81609-34-9 CAPLUS
CN Adenosine 5'-(hexahydrogen pentaphosphate), 8-(ethylthio)-, P''''→5'-ester with adenosine, pentasodium salt (9CI) (CA INDEX NAME)

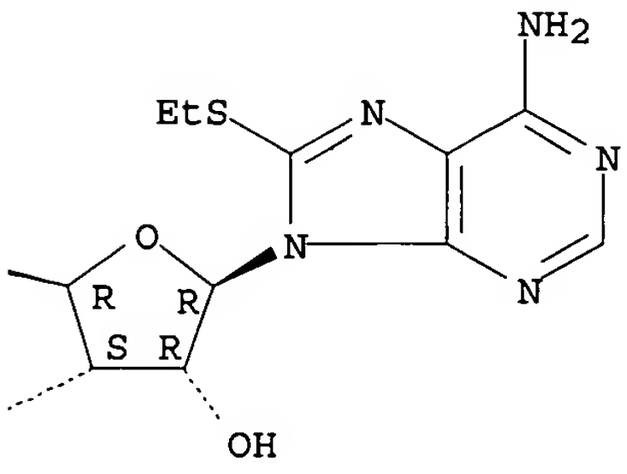
Absolute stereochemistry.

PAGE 1-A



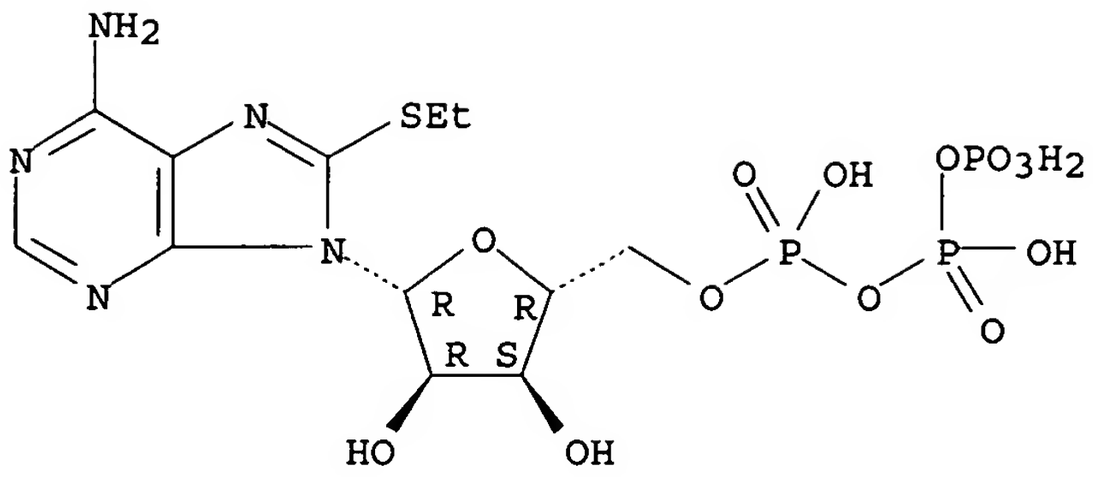
●5 Na

PAGE 1-B



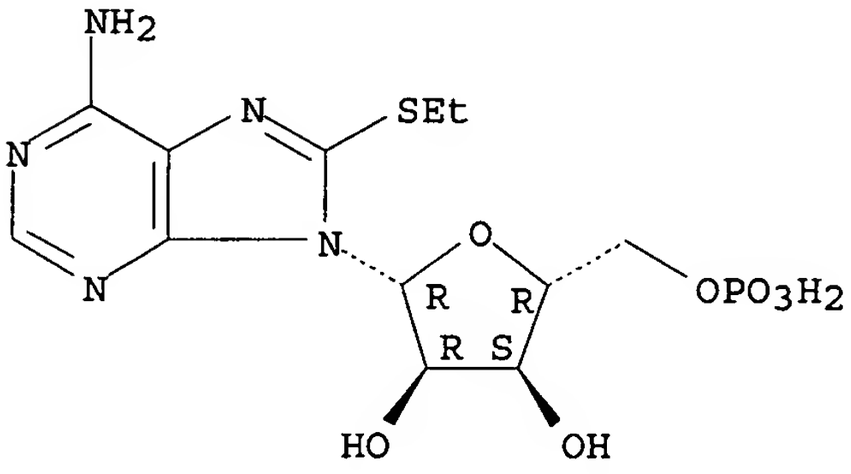
RN 81609-35-0 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(ethylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 81609-36-1 CAPLUS
CN 5'-Adenylic acid, 8-(ethylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

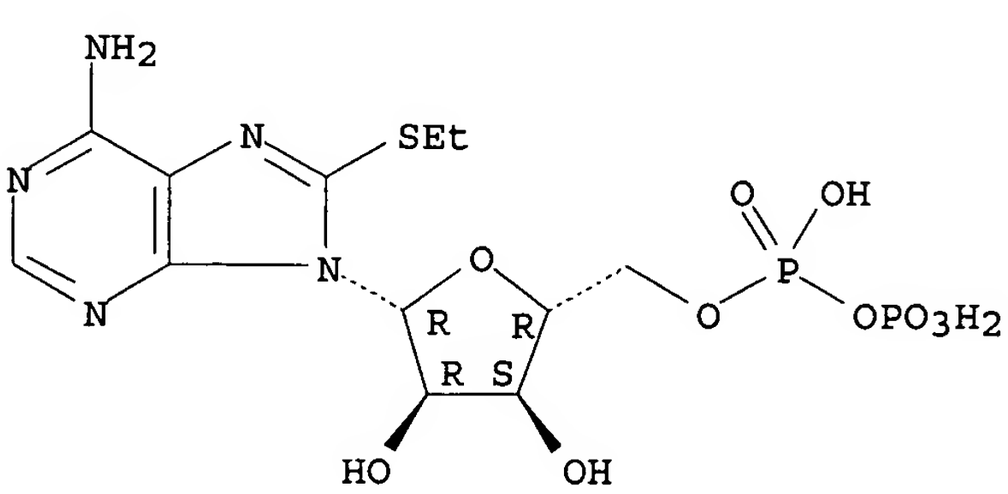


IT **81609-46-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with tributylammonium adenosine trimetaphosphate)
RN 81609-46-3 CAPLUS
CN Adenosine 5'-(trihydrogen diphosphate), 8-(ethylthio)-, compd. with N,N-dibutyl-1-butanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

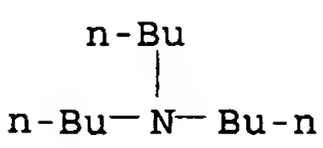
CRN 81609-45-2
CMF C12 H19 N5 O10 P2 S

Absolute stereochemistry.

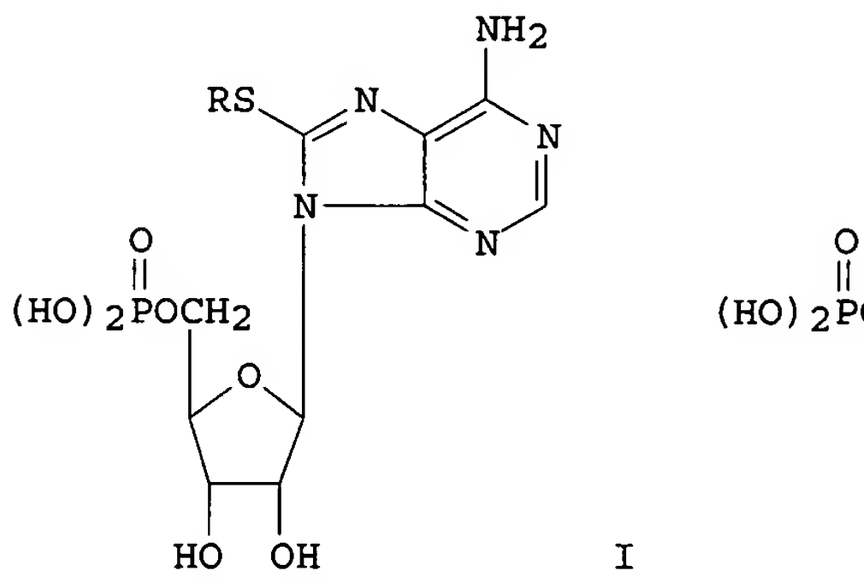


CM 2

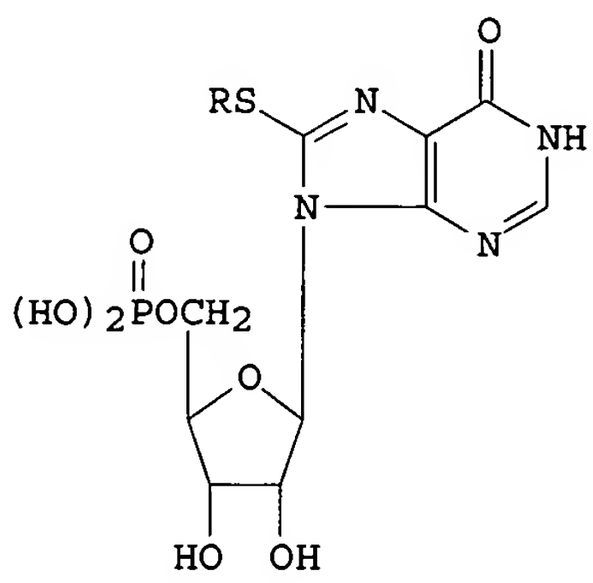
CRN 102-82-9
CMF C12 H27 N



L8 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1981:525864 CAPLUS
DN 95:125864
TI Inhibition of inosinic acid dehydrogenase by 8-substituted purine nucleotides
AU Skibo, Edward B.; Meyer, Rich B., Jr.
CS Sch. Pharm., Univ. California, San Francisco, CA, 94143, USA
SO Journal of Medicinal Chemistry (1981), 24(10), 1155-61
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
GI



I



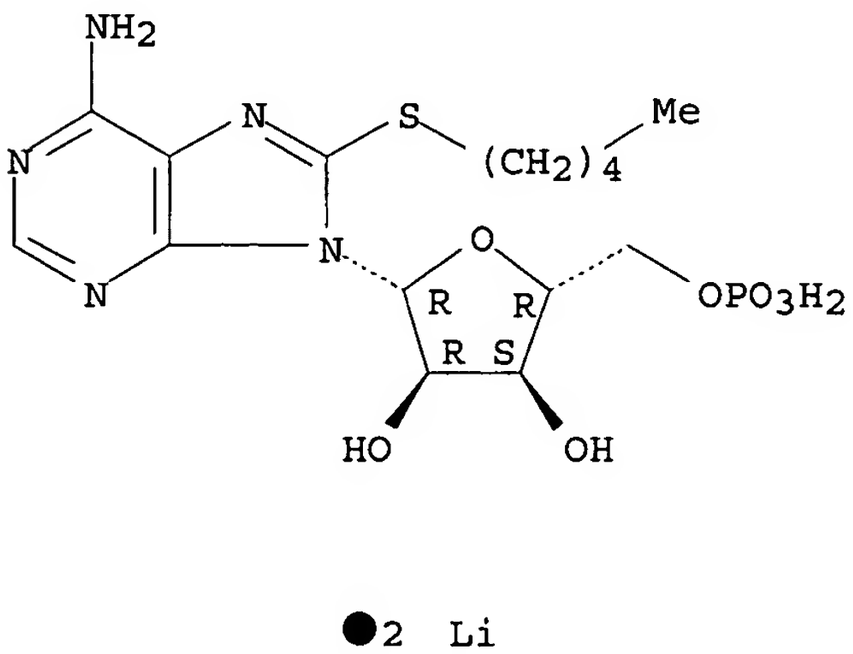
II

AB Twenty-seven AMP and IMP derivs. I and II (R = CH2Ph, substituted benzyl, CH2CH2Ph, etc.) were synthesized and studied for Escherichia coli IMP dehydrogenase (EC 1.2.1.14) [9028-93-7] inhibiting activity. Many inhibitors of this enzyme have anticancer activity. All of the compds. studied were competitive inhibitors in IMP-dependent competition studies and lacked substrate activity. Multiple regression anal. showed that for I and II (R = para substituted benzyl), the electron-withdrawing ability of the substituent on the benzylthio moiety correlated best with the Ki of the analogs.

IT **78710-82-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and IMP dehydrogenase inhibition by, antitumor activity in relation to)

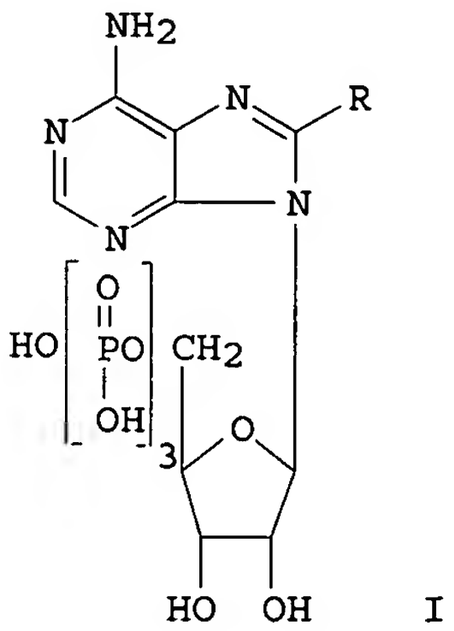
RN 78710-82-4 CAPLUS
CN 5'-Adenylic acid, 8-(pentylthio)-, dilithium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 Li

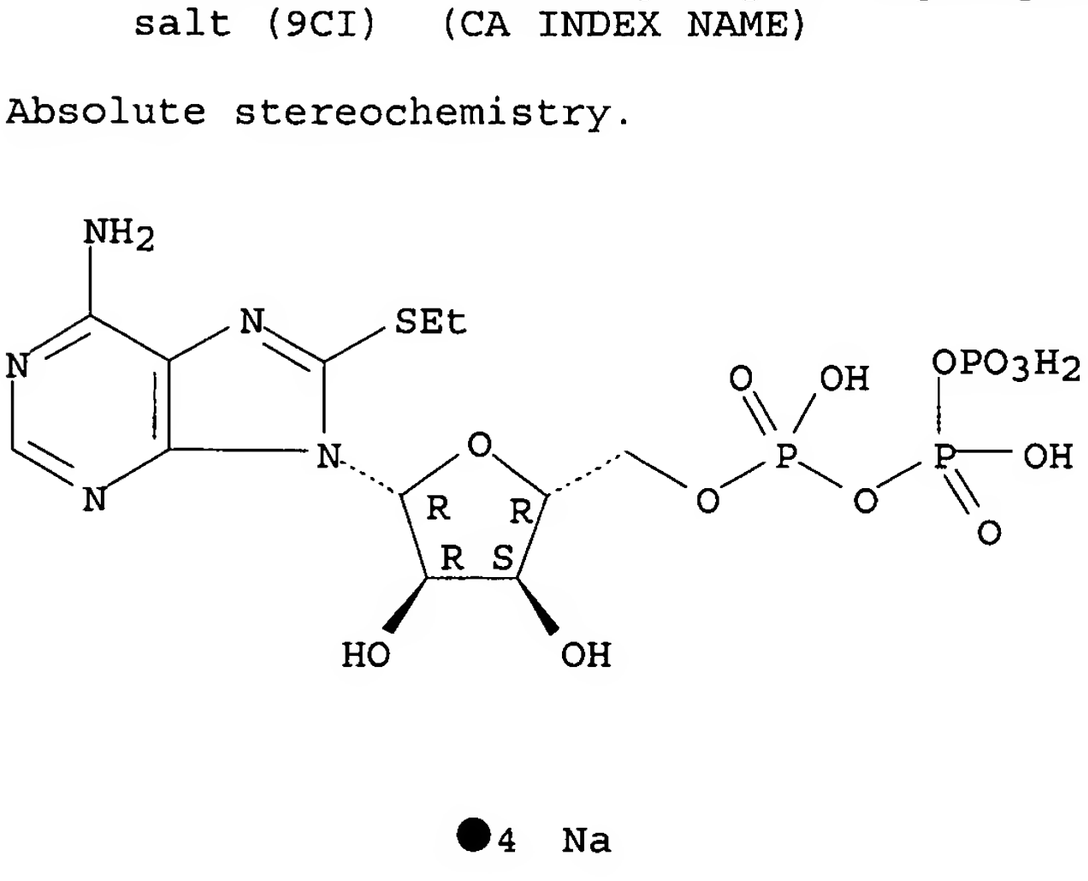
L8 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1979:604203 CAPLUS
DN 91:204203
TI Design of species- or isozyme-specific enzyme inhibitors. 3. Species and isozymic differences between mammalian and bacterial adenylate kinases in substituent tolerance in an enzyme-substrate complex
AU Hampton, Alexander; Picker, Donald
CS Fox Chase Cancer Cent., Inst. Cancer Res., Philadelphia, PA, 19111, USA
SO Journal of Medicinal Chemistry (1979), 22(12), 1529-32
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
GI



I

AB The ATP derivs. I (R = alkylthio, hydroxyalkylthio, or PhS) were prepared from tetra-Li 8-bromoadenosine 5'-triphosphate [71683-13-1] and the appropriate mercaptide and converted to the tetra Na salts. I and N6-ATP derivs. were evaluated as potential species- or isoenzyme-selective inhibitors of bacterial and mammalian adenylate kinase [9013-02-9]. The substituent attached at either N6 or C-8 influenced the affinity of the compds. for the enzymic ATP sites in both a species- and an isoenzyme-selective manner. Structure-activity relations are discussed.
IT **71683-14-2P 71683-15-3P 71683-16-4P**
71683-17-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and adenylate kinase-inhibiting activity of)
RN 71683-14-2 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(ethylthio)-, tetrasodium salt (9CI) (CA INDEX NAME)

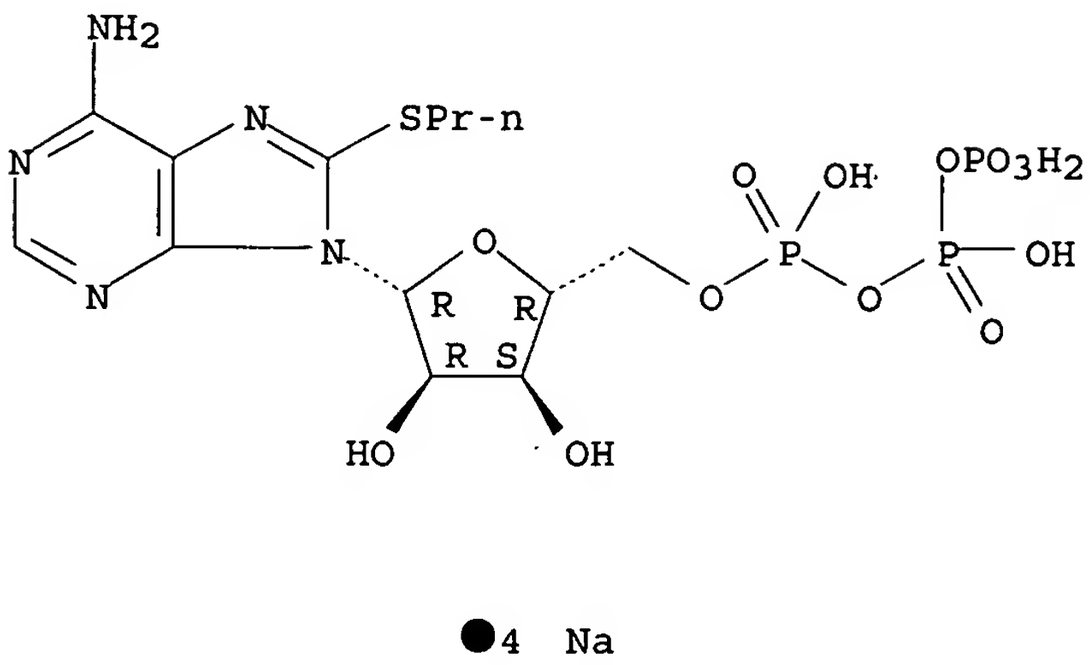
Absolute stereochemistry.



RN 71683-15-3 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(propylthio)-, tetrasodium

salt (9CI) (CA INDEX NAME)

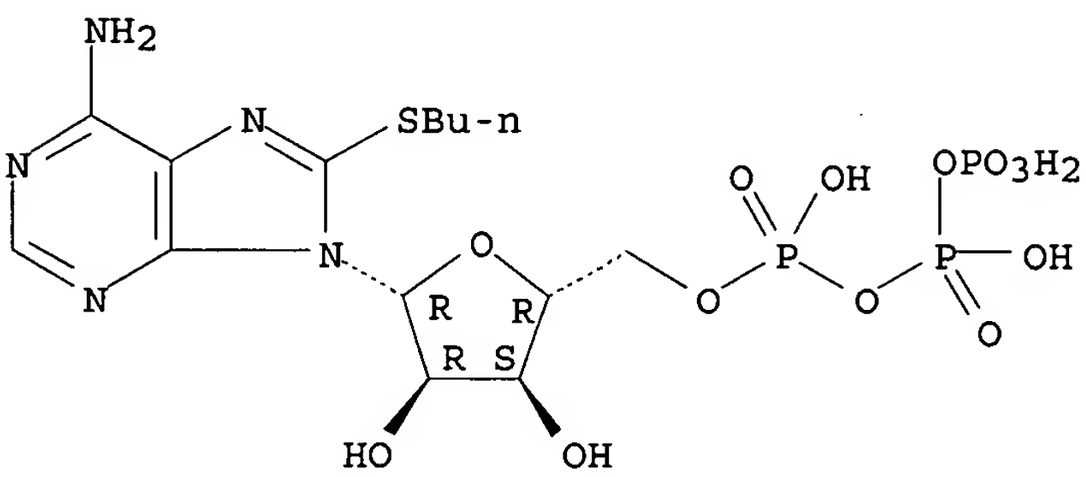
Absolute stereochemistry.



●4 Na

RN 71683-16-4 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)-, tetrasodium salt (9CI) (CA INDEX NAME)

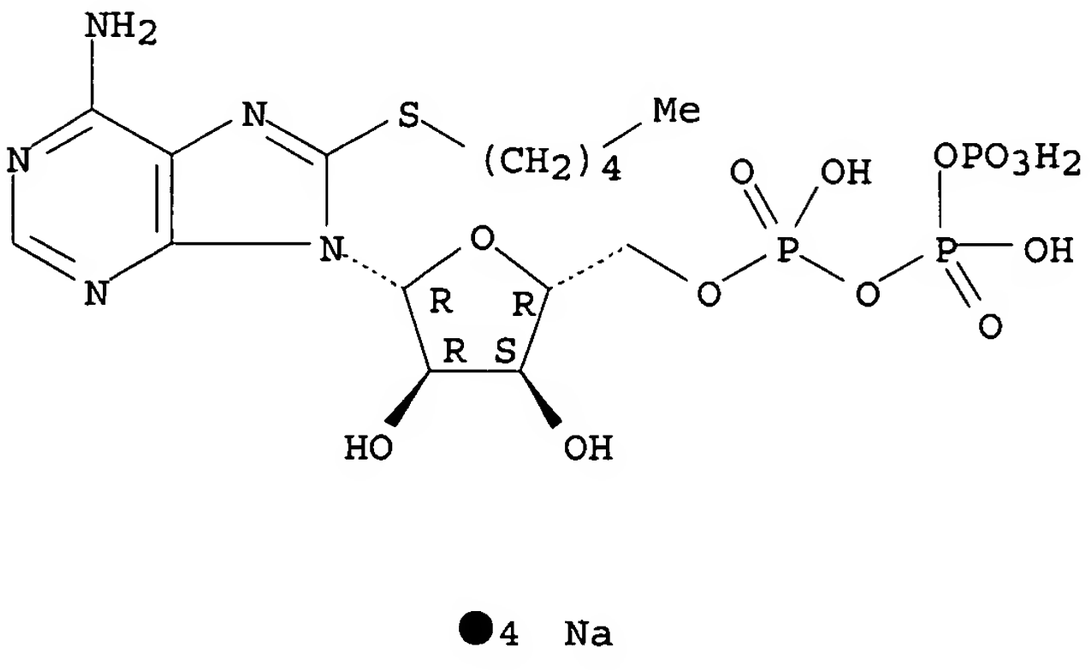
Absolute stereochemistry.



●4 Na

RN 71683-17-5 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(pentylthio)-, tetrasodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●4 Na

10/620,520

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1600txm

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS	4	FEB 21	STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS	5	FEB 22	The IPC thesaurus added to additional patent databases on STN
NEWS	6	FEB 22	Updates in EPFULL; IPC 8 enhancements added
NEWS	7	FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS	8	MAR 03	Updates in PATDPA; addition of IPC 8 data without attributes
NEWS	9	MAR 22	EMBASE is now updated on a daily basis
NEWS	10	APR 03	New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS	11	APR 03	Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL
NEWS	12	APR 04	STN AnaVist $500 visualization usage credit offered
NEWS	13	APR 12	LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS	14	APR 12	Improved structure highlighting in FQHIT and QHIT display in MARPAT
NEWS	15	APR 12	Derwent World Patents Index to be reloaded and enhanced during second quarter; strategies may be affected
NEWS	16	MAY 10	CA/CAplus enhanced with 1900-1906 U.S. patent records
NEWS	17	MAY 11	KOREAPAT updates resume
NEWS	18	MAY 19	Derwent World Patents Index to be reloaded and enhanced

NEWS EXPRESS FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT
http://download.cas.org/express/v8.0-Discover/

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available after June 2006

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* *

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* * * * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 12:31:35 ON 26 MAY 2006

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 12:31:43 ON 26 MAY 2006
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 25 MAY 2006 HIGHEST RN 885654-58-0
DICTIONARY FILE UPDATES: 25 MAY 2006 HIGHEST RN 885654-58-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

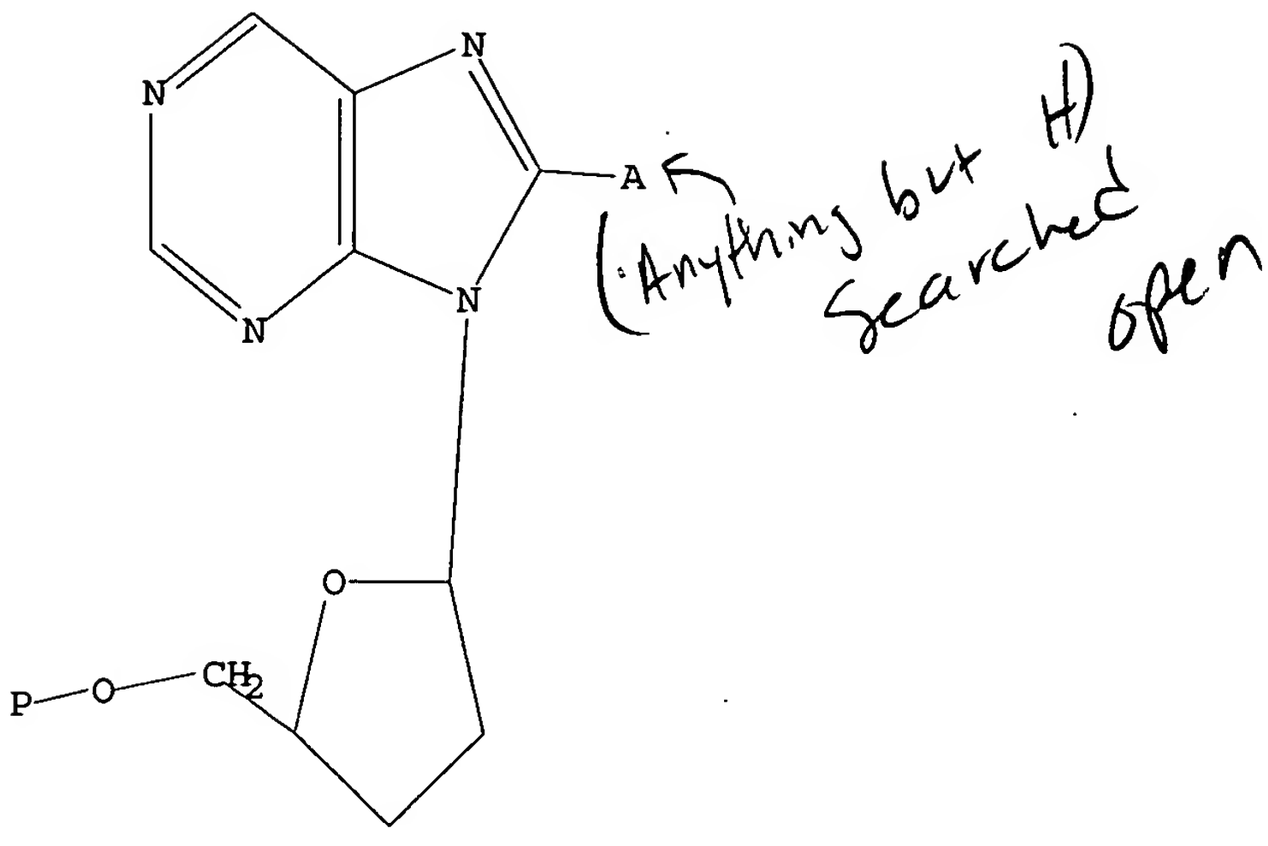
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10620520.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



(Anything but H)
Searched open

G1 Ak

Structure attributes must be viewed using STN Express query preparation.

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=> s l1 sam
SAMPLE SEARCH INITIATED 12:32:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     3555 TO ITERATE

 56.3% PROCESSED     2000 ITERATIONS                                 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        67525 TO    74675
PROJECTED ANSWERS:            1272 TO     2424

L2            50 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 12:32:11 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    73256 TO ITERATE

100.0% PROCESSED    73256 ITERATIONS                               1324 ANSWERS
SEARCH TIME: 00.00.01

L3          1324 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   166.94     167.15

FILE 'CAPLUS' ENTERED AT 12:32:17 ON 26 MAY 2006
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FILE COVERS 1907 - 26 May 2006 VOL 144 ISS 23
FILE LAST UPDATED: 25 May 2006 (20060525/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

```
=> s l3
L4          1225 L3

=> s ntpdase
             114 NTPDASE
              48 NTPDASES
L5           130 NTPDASE
                   (NTPDASE OR NTPDASES)

=> s nucleoside triphosphate diphosphohydrolase
           45789 NUCLEOSIDE
           30934 NUCLEOSIDES
           57166 NUCLEOSIDE
                   (NUCLEOSIDE OR NUCLEOSIDES)
           39515 TRIPHOSPHATE
           10190 TRIPHOSPHATES
           45662 TRIPHOSPHATE
                   (TRIPHOSPHATE OR TRIPHOSPHATES)
             442 DIPHOSPHOHYDROLASE
              50 DIPHOSPHOHYDROLASES
             452 DIPHOSPHOHYDROLASE
                   (DIPHOSPHOHYDROLASE OR DIPHOSPHOHYDROLASES)
L6           115 NUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE
                   (NUCLEOSIDE(W)TRIPHOSPHATE(W)DIPHOSPHOHYDROLASE)

=> s ectonucleotidase
             293 ECTONUCLEOTIDASE
             157 ECTONUCLEOTIDASES
L7           389 ECTONUCLEOTIDASE
                   (ECTONUCLEOTIDASE OR ECTONUCLEOTIDASES)

=> s atpdase
              58 ATPDASE
              15 ATPDASES
L8            60 ATPDASE
                   (ATPDASE OR ATPDASES)

=> s e-type atpase
         1936381 E
         1677630 TYPE
          580656 TYPES
         2126695 TYPE
                   (TYPE OR TYPES)
           81743 ATPASE
            7090 ATPASES
           82810 ATPASE
                   (ATPASE OR ATPASES)
L9            20 E-TYPE ATPASE
                   (E(W)TYPE(W)ATPASE)

=> s ecto atpase
            3357 ECTO
               2 ECTOS
            3359 ECTO
                   (ECTO OR ECTOS)
           81743 ATPASE
            7090 ATPASES
           82810 ATPASE
                   (ATPASE OR ATPASES)
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```
L10          457 ECTO ATPASE
                 (ECTO(W)ATPASE)

=> d his

     (FILE 'HOME' ENTERED AT 12:31:35 ON 26 MAY 2006)

     FILE 'REGISTRY' ENTERED AT 12:31:43 ON 26 MAY 2006
L1                STRUCTURE UPLOADED
L2             50 S L1 SAM
L3           1324 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 12:32:17 ON 26 MAY 2006
L4           1225 S L3
L5            130 S NTPDASE
L6            115 S NUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE
L7            389 S ECTONUCLEOTIDASE
L8             60 S ATPDASE
L9             20 S E-TYPE ATPASE
L10           457 S ECTO ATPASE

=> s l4 and (l5 or l6 or l7 or l8 or l9 or l10)
L11            11 L4 AND (L5 OR L6 OR L7 OR L8 OR L9 OR L10)

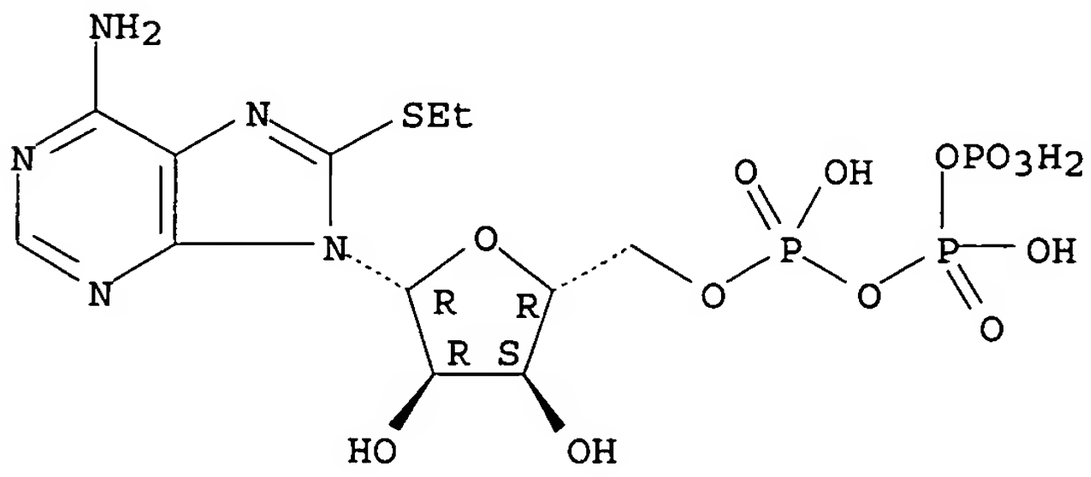
=> d bib abs hitstr 1-11 l11

L11  ANSWER 1 OF 11  CAPLUS  COPYRIGHT 2006 ACS on STN
AN   2004:911398  CAPLUS
DN   142:214281
TI   C8-substituted purine nucleotide analogs and their use as inhibitors of
     nucleoside triphosphate diphosphohydrolases
IN   Halbfinger, Efrat; Fischer, Bilha; Beaudoin, Adrien R.; Gendron, Fernand
     Pierre
PA   Universite de Sherbrooke, Can.; Bar-Ilan University
SO   Can. Pat. Appl., 54 pp.
     CODEN: CPXXEB
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.           KIND   DATE        APPLICATION NO.          DATE
     ---------------      ----   --------    --------------------     --------
PI   CA 2311084            AA    20011209    CA 2000-2311084          20000609
PRAI CA 2000-2311084               20000609
OS   CASREACT 142:214281
AB   Ectonucleoside triphosphate diphosphohydrolases [NTPDases; EC
     3.6.1.5] constitute a family of enzymes which are involved in the metabolism
     of extracellular nucleotides, catalyzing the hydrolysis of the gamma and
     beta phosphate bonds of triphospho- and diphosphonucleosides (whereas
     5'-nucleotidases [EC 3.1.3.5] catalyze the hydrolysis of alpha phosphate
     bond of monophosphonucleosides). These extracellular nucleotides interact
     with endothelial, epithelial and smooth muscle cells, as well as blood
     cells and lymphoid cells, to influence the different physiol. systems of
     vertebrates. Since these ecto-nucleotidases alter the extracellular
     concns. of nucleotides these enzymes modulate their physiol. effects,
     including, for example, platelet aggregation, heart function, control of
     vascular tone and inflammation reactions, electrolyte secretion and
     gastrointestinal motility, neurotransmission both in central and
     peripheral nervous systems, as well as other effects in other physiol.
     systems. This invention provides C8 substituted purine nucleotide
     analogs, such as ATP analogs, and further provides their use as inhibitors
     of NTPDases and thereby as tools to modulate the conversion of
     nucleotides into nucleoside derivs., and thus modulate the levels of these
     compds. Such modulation further provides for the modulation of the
     activity and function of many processes which are affected by these
     compds.
IT   81609-35-0P 284040-51-3P 284040-52-4P
     284040-53-5P
     RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);
     SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
```

study); PREP (Preparation); USES (Uses)
(C8-substituted purine nucleotide analogs and their use as inhibitors of **nucleoside triphosphate diphosphohydrolases** to modulate purine nucleotide levels and biol. processes)

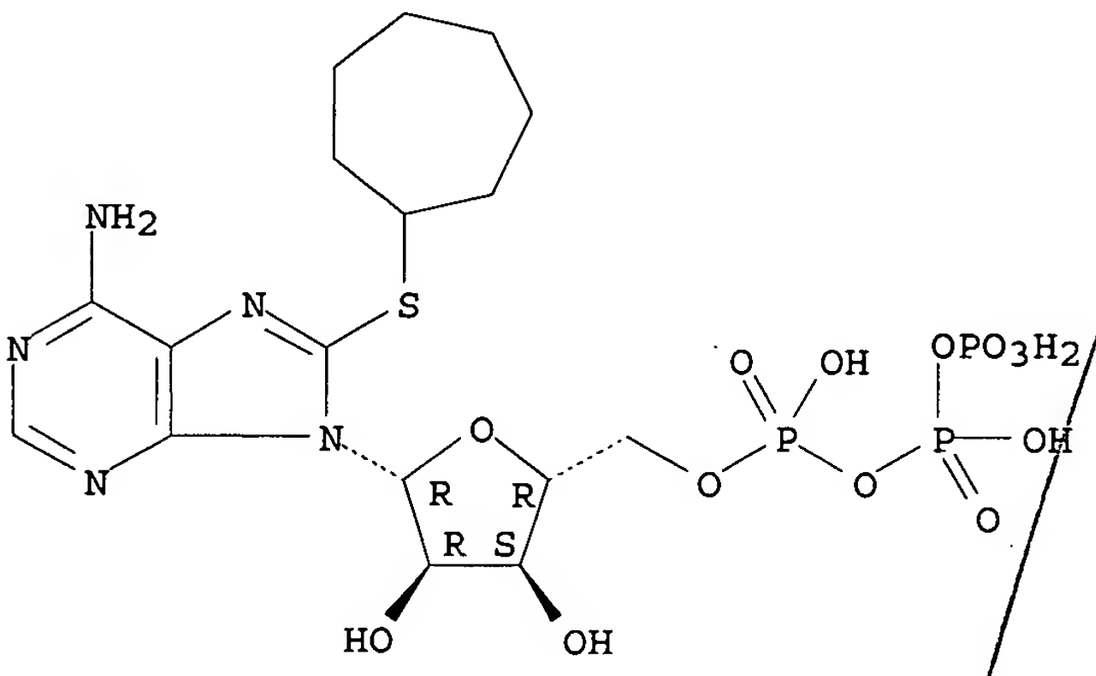
RN 81609-35-0 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(ethylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



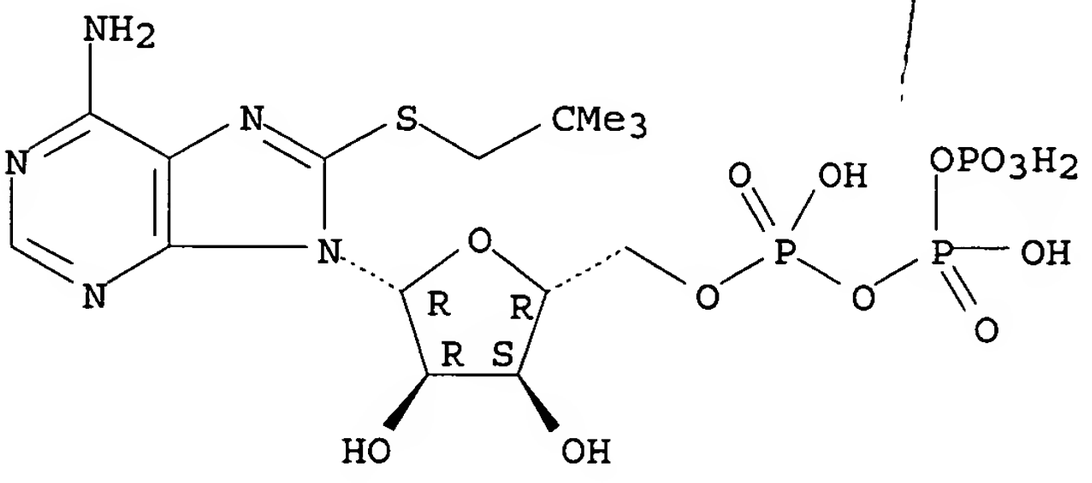
RN 284040-51-3 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(cycloheptylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



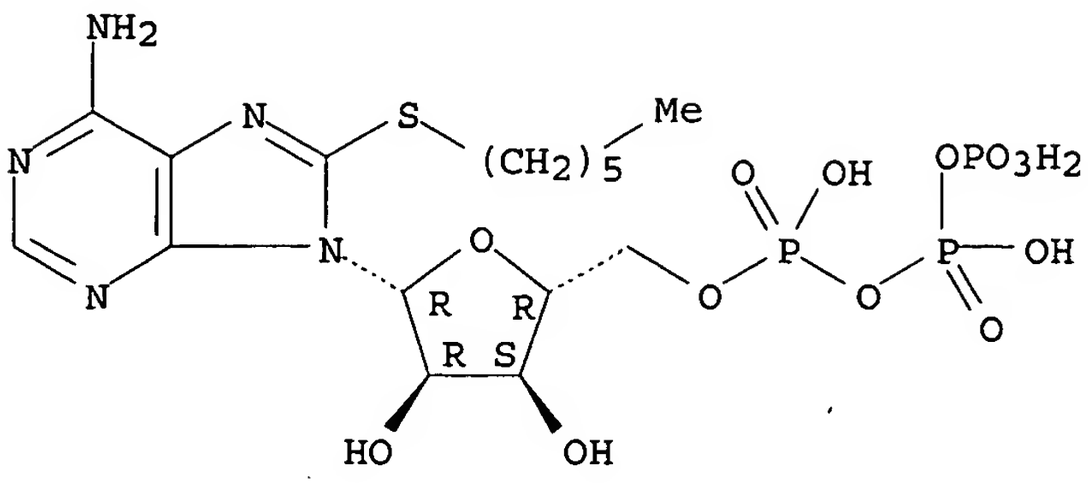
RN 284040-52-4 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-[(2,2-dimethylpropyl)thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



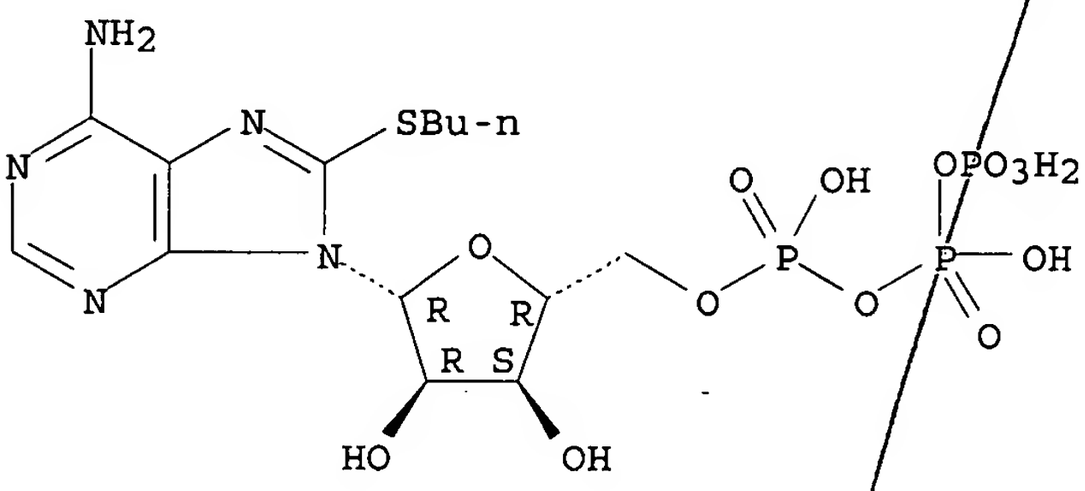
RN 284040-53-5 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(hexylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



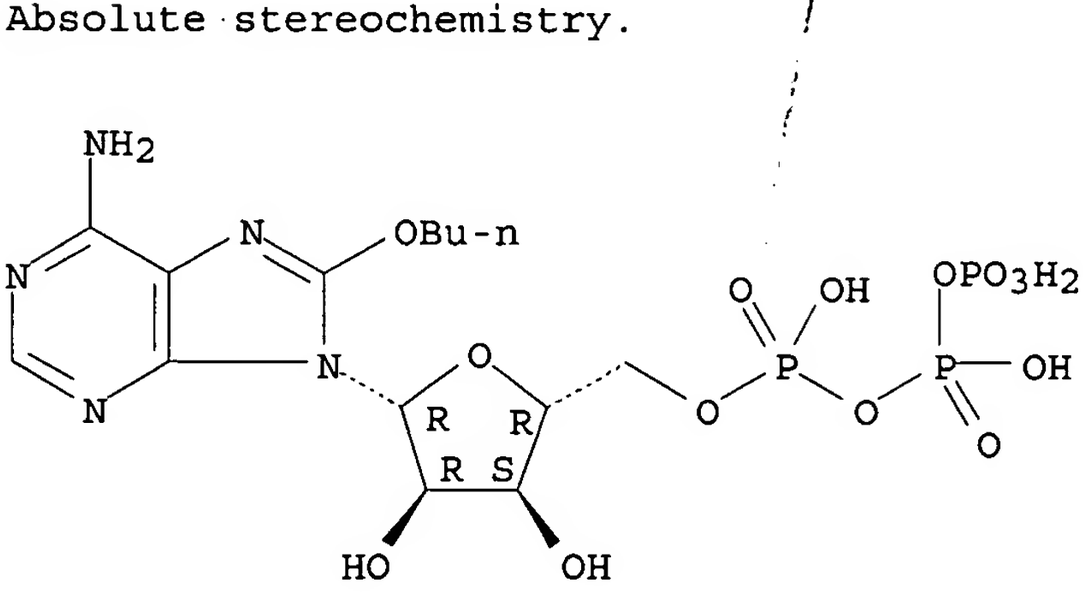
IT **284040-54-6 284040-60-4**
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(C8-substituted purine nucleotide analogs and their use as inhibitors of **nucleoside triphosphate diphosphohydrolases** to modulate purine nucleotide levels and biol. processes)
RN 284040-54-6 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



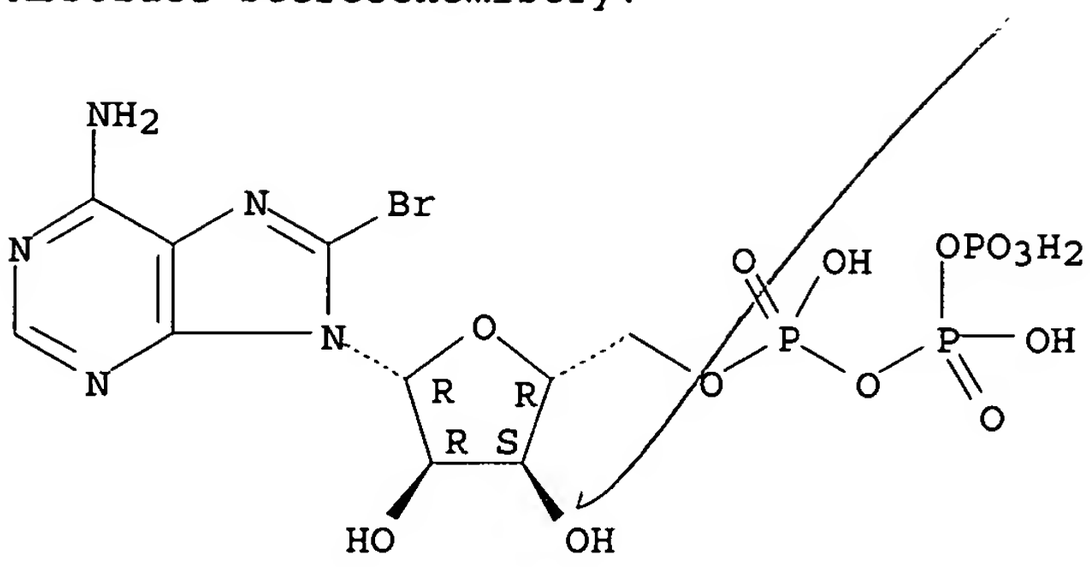
RN 284040-60-4 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-butoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **23567-97-7**, 8-Bromo-ATP
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(substrate; C8-substituted purine nucleotide analogs and their use as inhibitors of **nucleoside triphosphate diphosphohydrolases** to modulate purine nucleotide levels and biol. processes)
RN 23567-97-7 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-bromo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L11 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:856092 CAPLUS
DN 139:333119
TI Ecto-**nucleoside triphosphate diphosphohydrolase** inhibition-based methods for screening for a compound useful in the treatment or prevention of lymphocytic disorders, for inhibiting lymphocyte activity and preventing or treating lymphocytic disorders
IN Beaudoin, Adrien; Benrezzak, Ouhida
PA Bioflash Inc., Can.
SO PCT Int. Appl., 63 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003089664	A1	20031030	WO 2003-CA583	20030422
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	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2382768	AA	20031019	CA 2002-2382768	20020419
	CA 2479501	AA	20031030	CA 2003-2479501	20030422
	AU 2003226989	A1	20031103	AU 2003-226989	20030422
	US 2005164306	A1	20050728	US 2003-511133	20030422
PRAI	CA 2002-2382768	A	20020419		
	WO 2003-CA583	W	20030422		

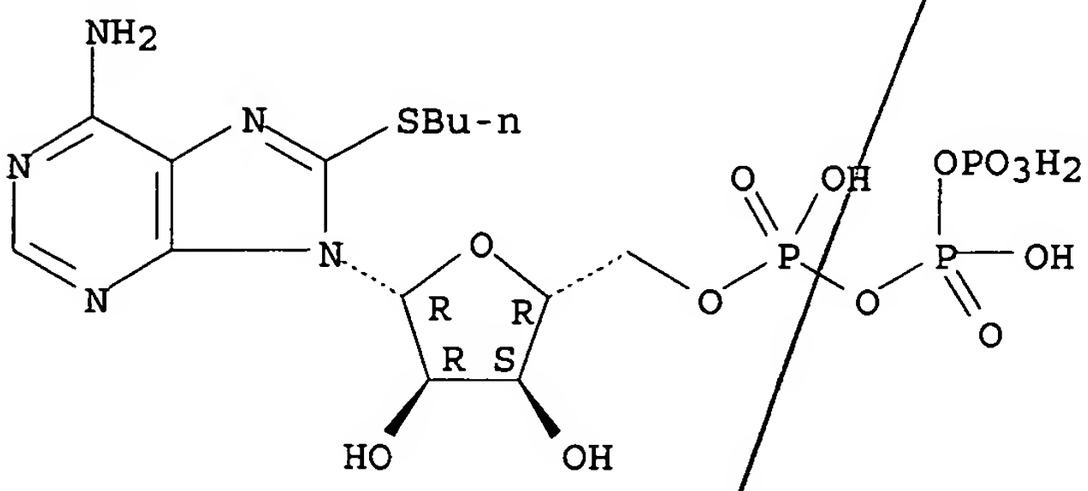
AB The invention discloses a method of screening for a compound useful in the treatment of a disease or condition characterized by an immune cell disorder, wherein the cell expresses ecto-**nucleoside triphosphate diphosphohydrolases** (**NTPDases**), the method comprising contacting a candidate compound with **NTPDase**, wherein the candidate compound is selected if the activity of the **NTPDase** is reduced in the presence of the candidate compound as compared to that in the absence thereof. The invention also discloses a method for inhibiting an immune cell activity in a mammal, comprising targeting immune cells with an effective amount of a **NTPDase** inhibitor. The invention further discloses a method to prevent or reduce the risk of rejection of transplanted tissue or organ, comprising administering to the animal an effective amount of **NTPDase** inhibitor.

IT **284040-54-6 344402-39-7**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(ecto-**nucleoside triphosphate**

diphosphohydrolase inhibition-based methods for screening for agents for treatment of immune cell disorder-associated conditions)

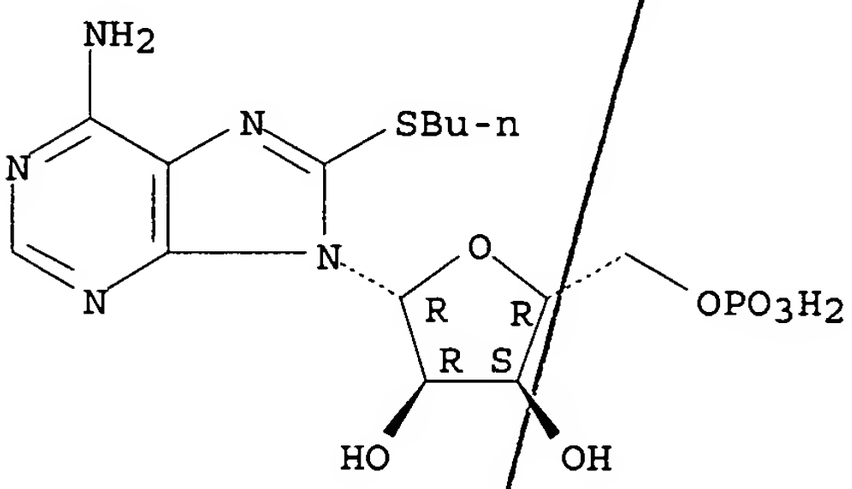
RN 284040-54-6 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 344402-39-7 CAPLUS
CN 5'-Adenylic acid, 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



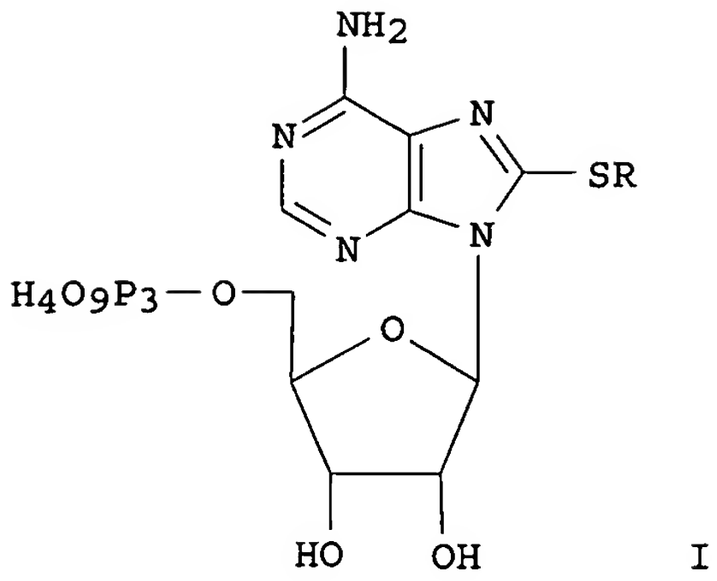
RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:711173 CAPLUS
DN 139:230955
TI Preparation of C8-substituted purine nucleotide analogs as **NTPDase** inhibitors
IN Beaudoin, Adrien R.; Gendron, Fernand-Pierre; Halbfinger, Efrat; Fischer, Bilha
PA Bar-Ilan University, Israel; Universite De Sherbrooke
SO U.S., 21 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6617439	B1	20030909	US 2000-591177	20000609
	US 2004043955	A1	20040304	US 2003-620520	20030716
PRAI	US 2000-591177	A3	20000609		

OS MARPAT 139:230955
GI

Parent Case



I

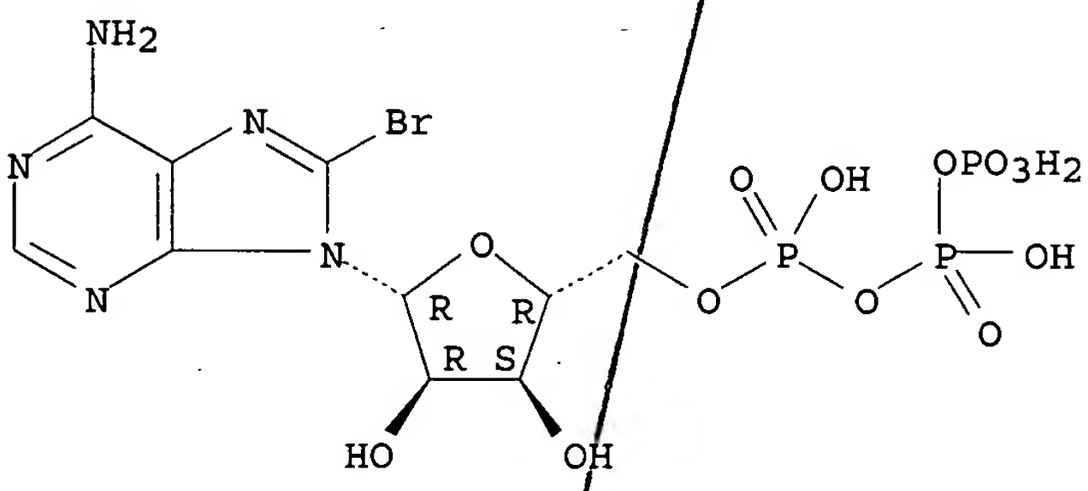
AB C8-substituted purine nucleotide analogs, I (R is alkyl, cycloalkyl) such as ATP analogs, and their use is described, including their use as inhibitors of **NTPDases** and thereby as tools to modulate the conversion of nucleotides into nucleoside derivs., and thus modulate the levels of these compds. Such modulation further provides for the modulation of the activity and function of many processes which are affected by these compds. Thus, I [R = (CH2)3Me] was prepared and tested in vivo as NTDPase inhibitor. I [R = (CH2)3Me] interacts specifically with the binding site of the enzyme potentially reduces the risk of interference with other ATP-binding enzymes or receptors, and thus possesses a high degree of specificity. The compds. of the invention were analyzed with resp. to any effects on the activity of purinoceptors.

IT **23567-97-7**, 8-Bromoadenosine triphosphate
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of C8-substituted purine nucleotide analogs as **NTPDase** inhibitors)

RN 23567-97-7 CAPLUS

CN Adenosine 5'-(tetrahydrogen triphosphate), 8-bromo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

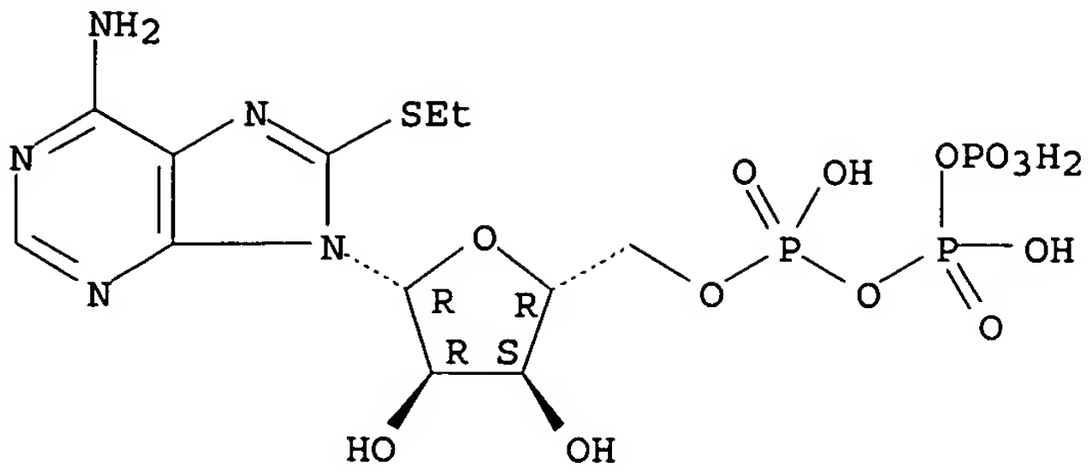


IT **81609-35-0P 284040-51-3P 284040-52-4P**
284040-53-5P 284040-54-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of C8-substituted purine nucleotide analogs as **NTPDase** inhibitors)

RN 81609-35-0 CAPLUS

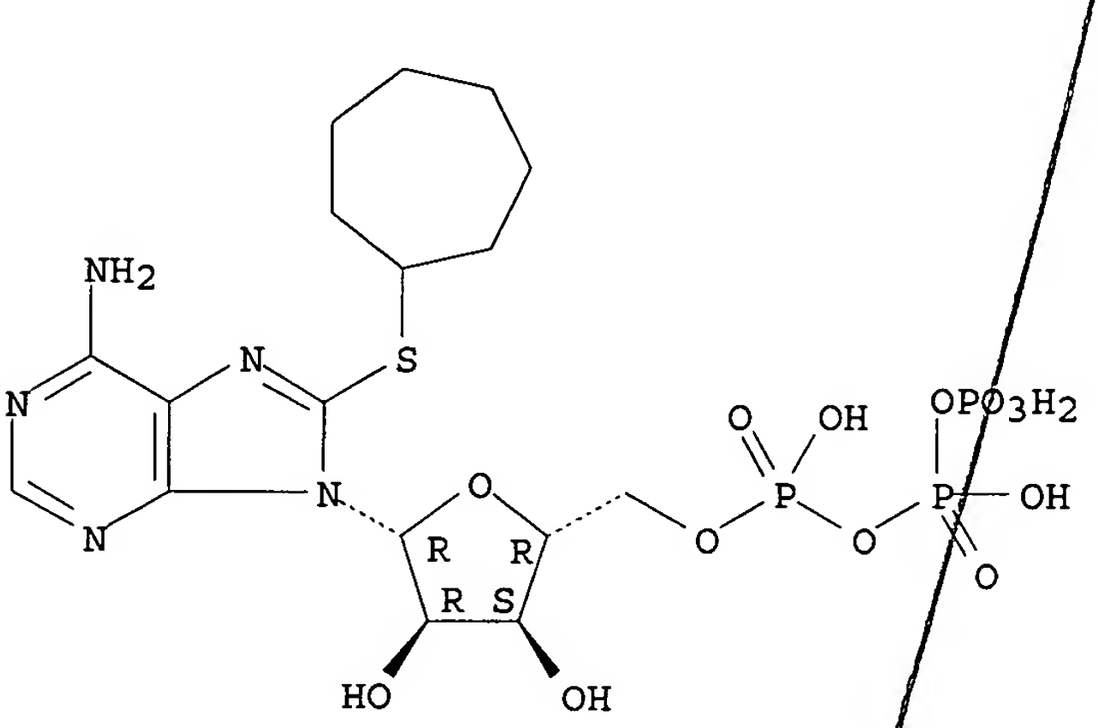
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(ethylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



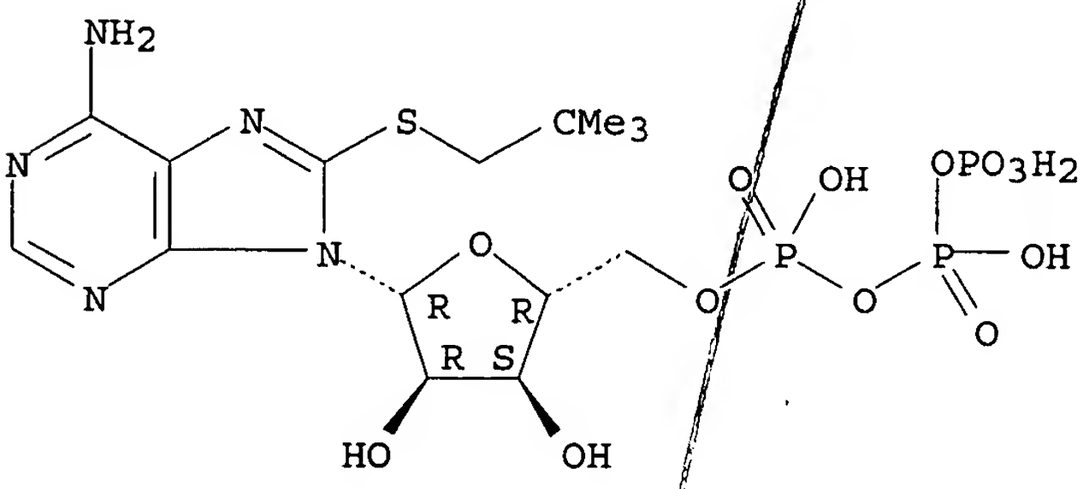
RN 284040-51-3 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(cycloheptylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



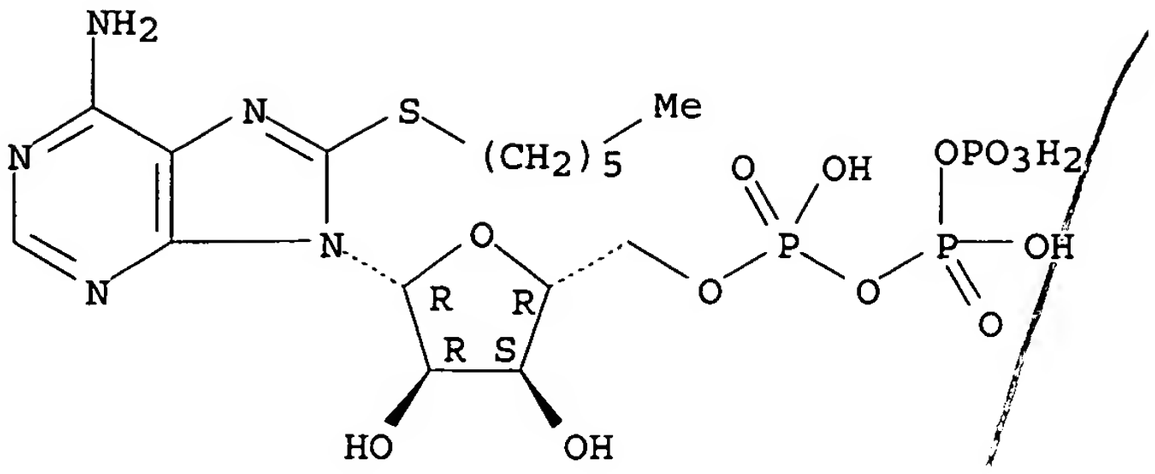
RN 284040-52-4 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-[(2,2-dimethylpropyl)thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



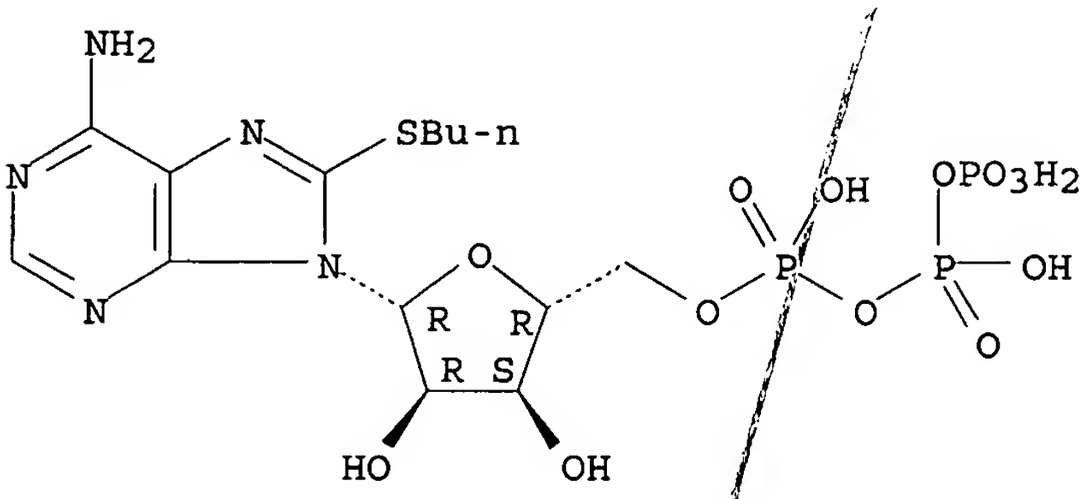
RN 284040-53-5 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(hexylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



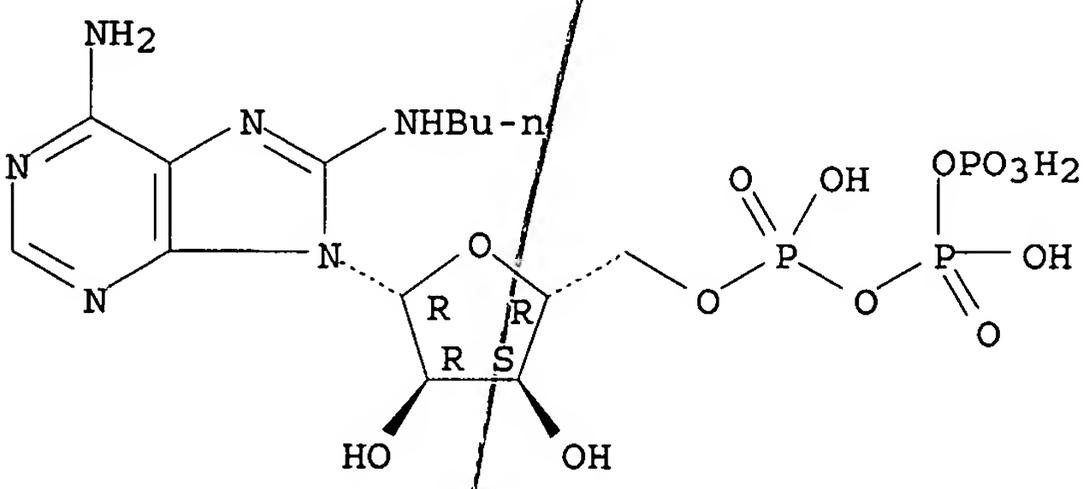
RN 284040-54-6 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



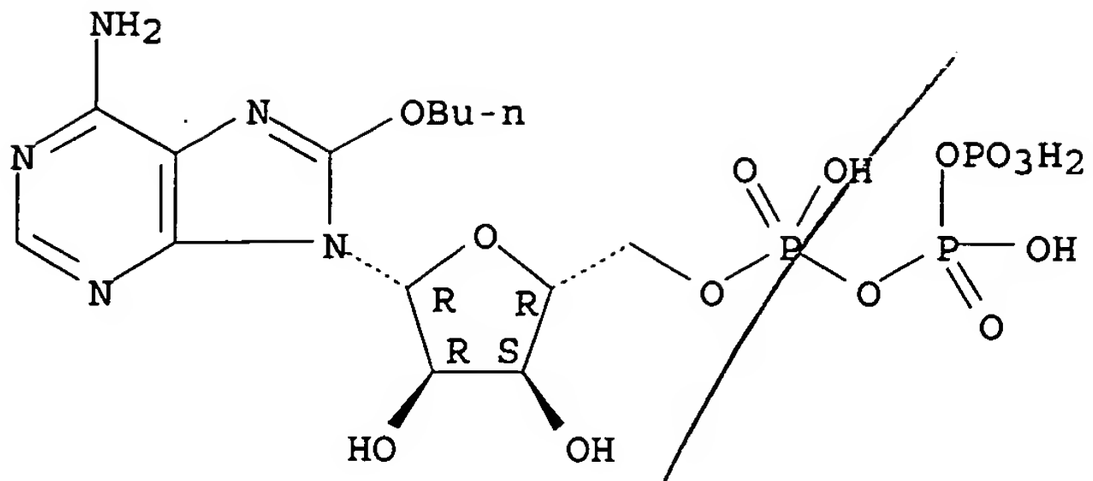
IT **284040-59-1 284040-60-4**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of C8-substituted purine nucleotide analogs as **NTPDase** inhibitors)
RN 284040-59-1 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylamino)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 284040-60-4 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-butoxy- (9CI) (CA INDEX NAME)

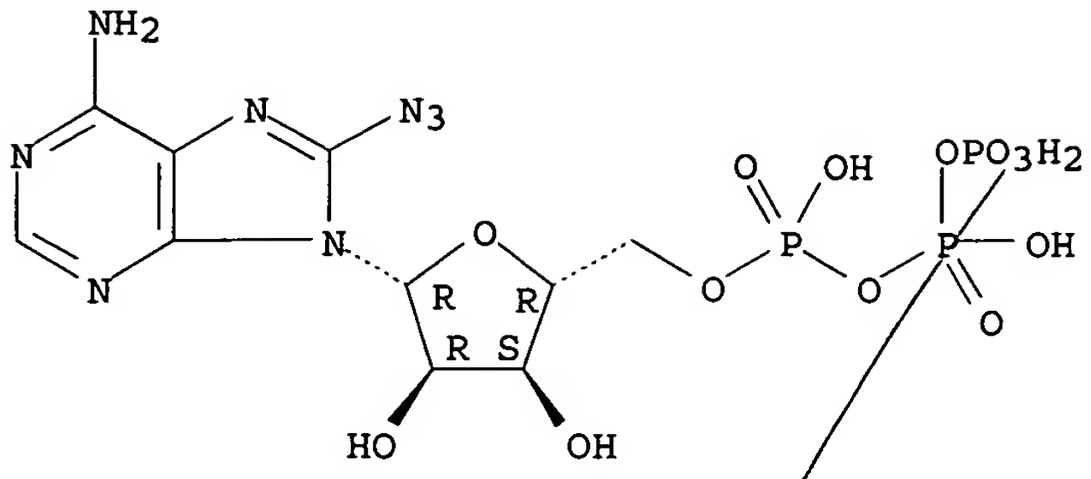
Absolute stereochemistry.



RE.CNT 71 THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2002:910711 CAPLUS
DN 138:232038
TI Heteromultimerization modulates P2X receptor functions through participating extracellular and C-terminal subdomains
AU Koshimizu, Taka-aki; Ueno, Susumu; Tanoue, Akito; Yanagihara, Nobuyuki; Stojilkovic, Stanko S.; Tsujimoto, Gozoh
CS Department of Molecular and Cell Pharmacology, National Institutes of Health, NICHD, Bethesda, MD, 20892, USA
SO Journal of Biological Chemistry (2002), 277(49), 46891-46899
CODEN: JBCHA3; ISSN: 0021-9258
PB American Society for Biochemistry and Molecular Biology
DT Journal
LA English
AB P2X purinergic receptors (P2XRs) differ among themselves with respect to their ligand preferences and channel kinetics during activation, desensitization, and recovery. However, the contributions of distinct receptor subdomains to the subtype-specific behavior have been incompletely characterized. Homomeric receptors having the extracellular domain of the P2X3 subunit in the P2X2a-based backbone (P2X2a/X3ex) mimicked two intrinsic functions of P2X3R, sensitivity to αβ-methylene ATP and **ecto-ATPase**-dependent recovery from endogenous desensitization; these two functions were localized to the N- and C-terminal halves of the P2X3 extracellular loop, resp. The chimeric P2X2aR/X3ex receptors also desensitized with accelerated rates compared with native P2X2aR, and the introduction of P2X2 C-terminal splicing into the chimeric subunit (P2X2b/X3ex) further increased the rate of desensitization. Phys. and functional heteromerization of native P2X2a and P2X2b subunits was also demonstrated. In heteromeric receptors, the ectodomain of P2X3 was a structural determinant for ligand selectivity and recovery from desensitization, and the C terminus of P2X2 was an important factor for the desensitization rate. Furthermore, [γ-32P]8-azido ATP, a photoreactive agonist, was effectively crosslinked to P2X3 subunit in homomeric receptors but not in heteromeric P2X2 + P2X3Rs. These results indicate that heteromeric receptors formed by distinct P2XR subunits develop new functions resulting from integrative effects of the participating extracellular and C-terminal subdomains.
IT **53696-59-6**, 8-Azido ATP
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(heteromultimerization modulates P2X receptor functions through participating extracellular and C-terminal subdomains as studied in GT1 cells)
RN 53696-59-6 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-azido- (9CI) (CA INDEX NAME)

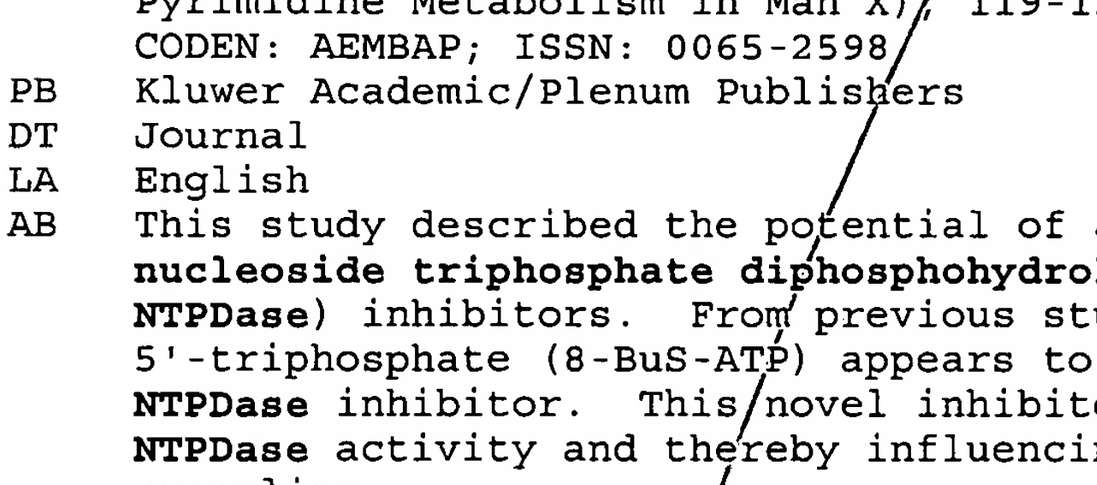
Absolute stereochemistry.



RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

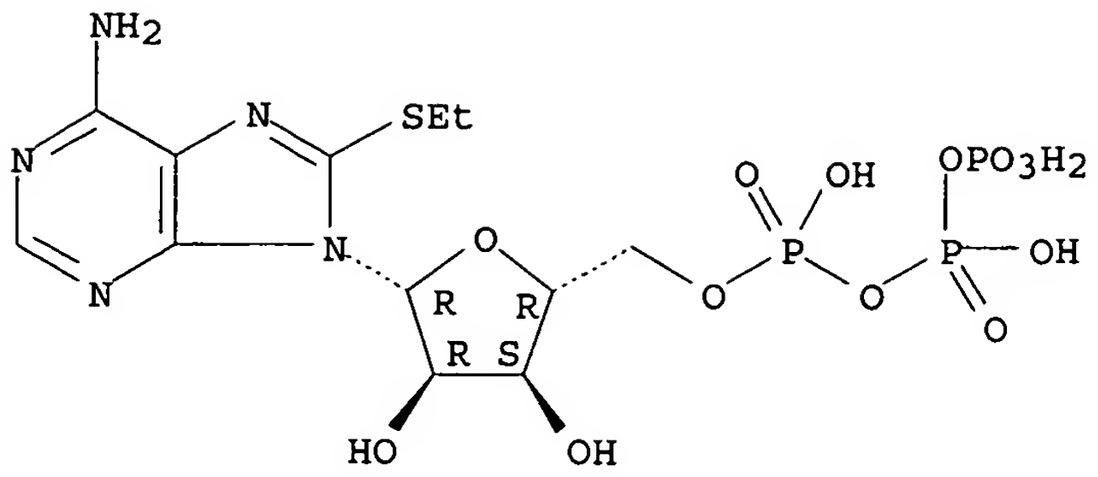
L11 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2001:327844 CAPLUS
DN 135:149038
TI Inhibitors of **NTPDase**: key players in the metabolism of extracellular purines
AU Gendron, F. P.; Halbfinger, E.; Fischer, B.; Beaudoin, A. R.
CS Department of Biology, University of Sherbrooke, Sherbrooke, Can.
SO Advances in Experimental Medicine and Biology (2000), 486(Purine and Pyrimidine Metabolism in Man X), 119-123
CODEN: AEMBAP; ISSN: 0065-2598
PB Kluwer Academic/Plenum Publishers
DT Journal
LA English
AB This study described the potential of a new class of ATP analogs as **nucleoside triphosphate diphosphohydrolase** (**NTPDase**) inhibitors. From previous studies, 8-thiobutyladenosine 5'-triphosphate (8-BuS-ATP) appears to be a specific and efficient **NTPDase** inhibitor. This novel inhibitor is a new tool to regulate **NTPDase** activity and thereby influencing purine signaling in mammalian.
IT **23567-97-7 81609-35-0 284040-51-3**
284040-53-5 284040-54-6 284040-59-1
284040-60-4 352690-39-2
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(inhibitors of **nucleoside triphosphate diphosphohydrolase** - key players in metabolism of extracellular purines)
RN 23567-97-7 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-bromo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



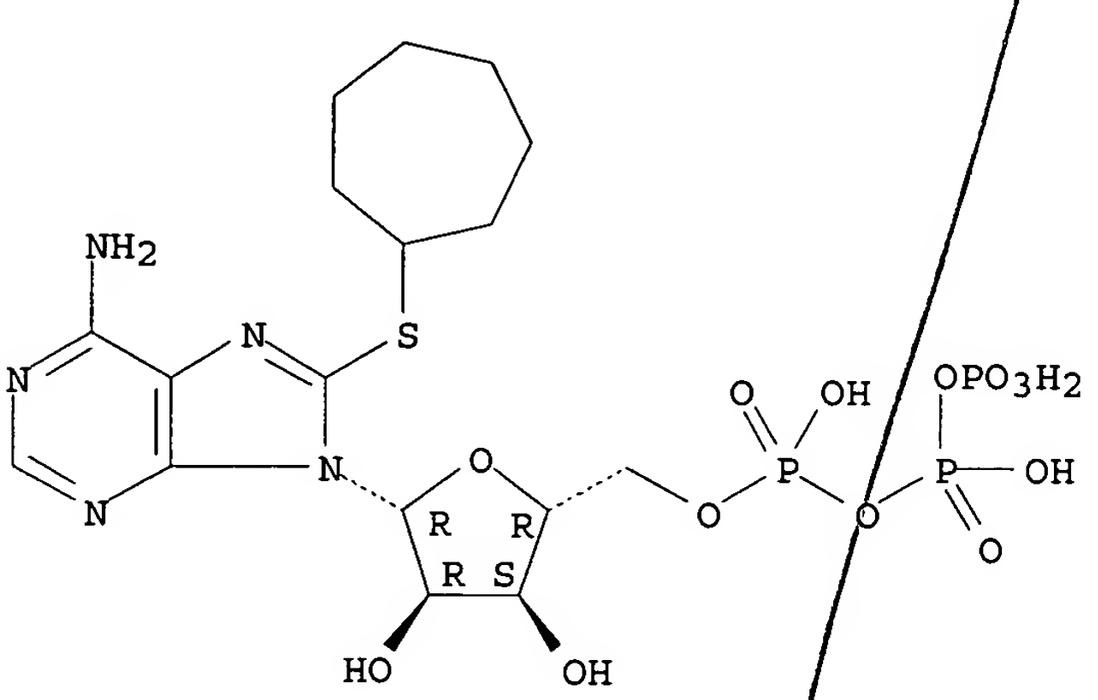
RN 81609-35-0 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(ethylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



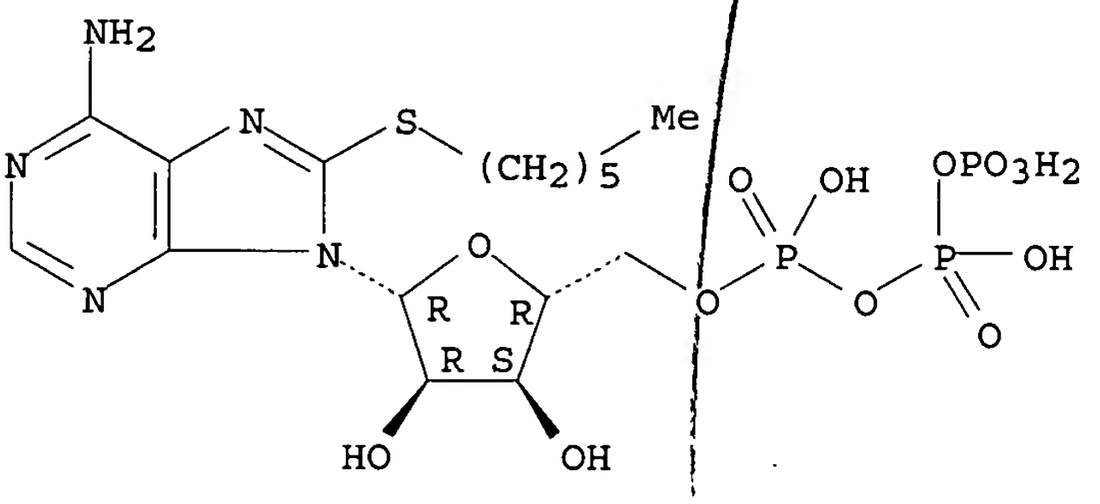
RN 284040-51-3 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(cycloheptylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



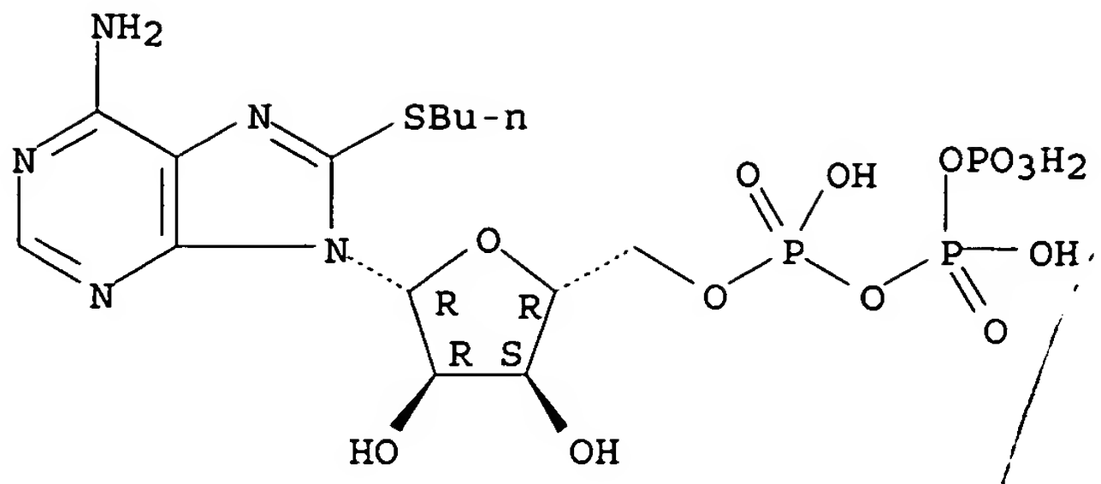
RN 284040-53-5 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(hexylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



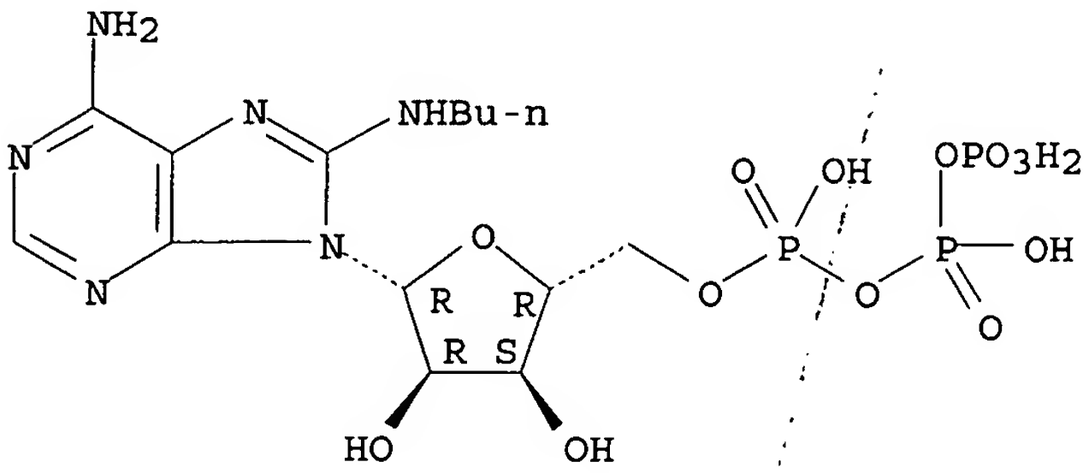
RN 284040-54-6 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



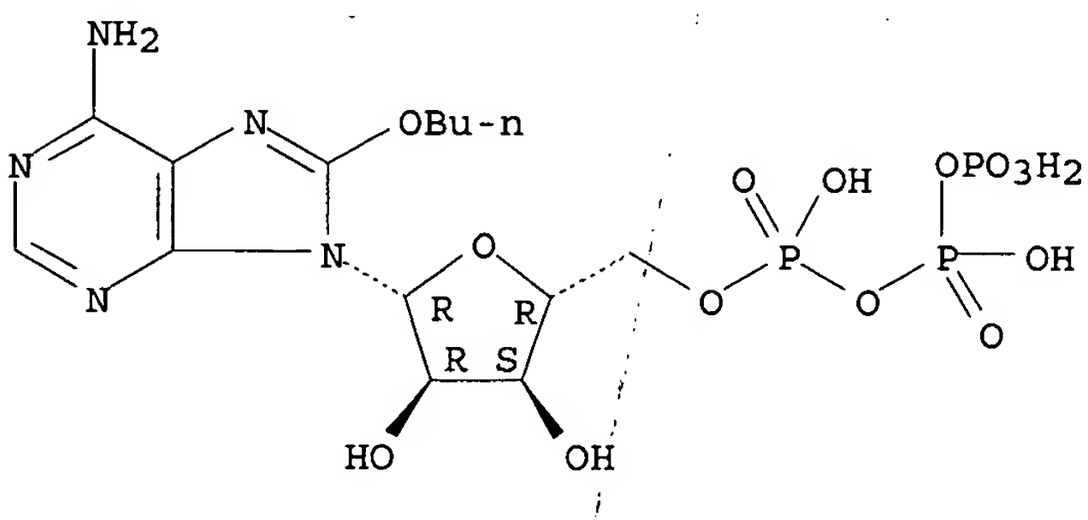
RN 284040-59-1 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylamino)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



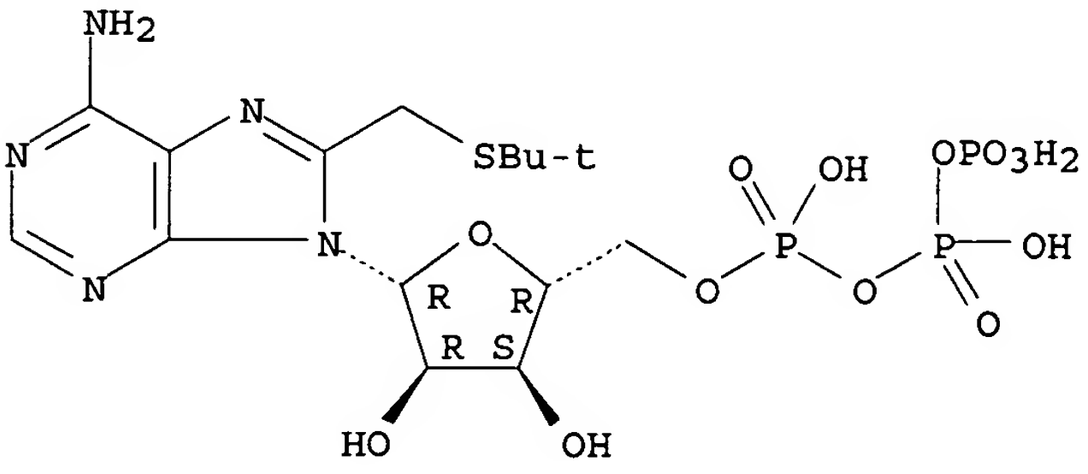
RN 284040-60-4 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-butoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 352690-39-2 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-[[(1,1-dimethylethyl)thio]methyl]- (9CI) (CA INDEX NAME)

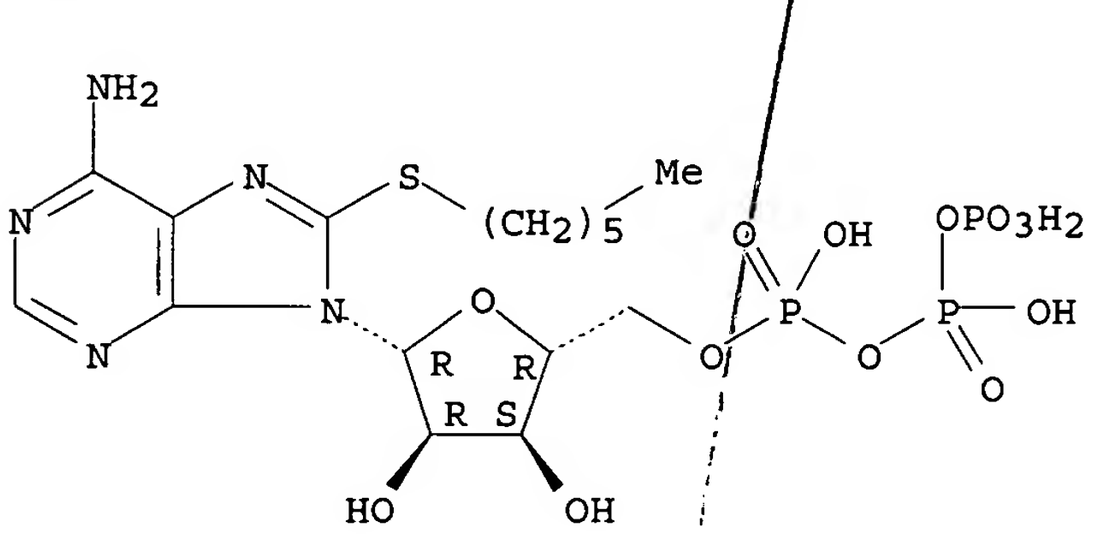
Absolute stereochemistry.



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

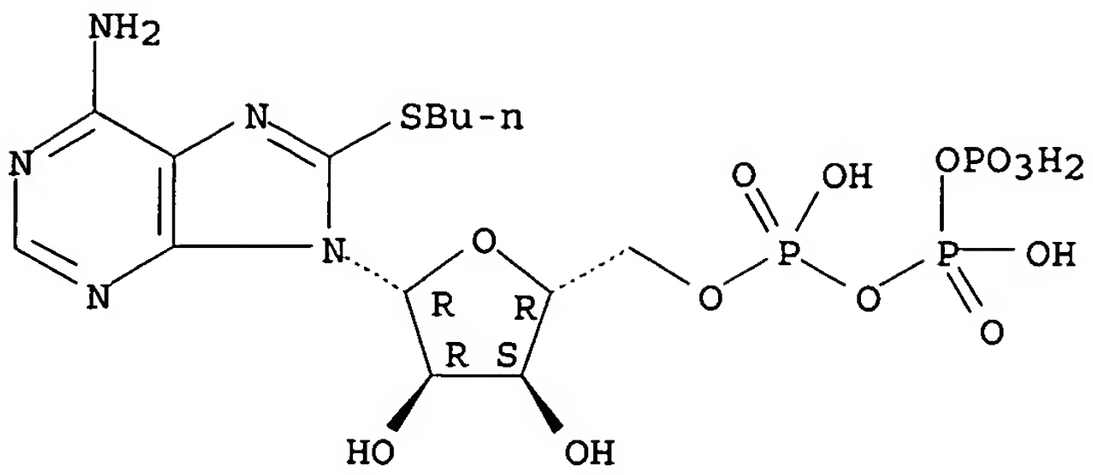
L11 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2000:304989 CAPLUS
DN 133:105244
TI Novel Inhibitors of **Nucleoside Triphosphate Diphosphohydrolases**: Chemical Synthesis and Biochemical and Pharmacological Characterizations
AU Gendron, Fernand-Pierre; Halbfinger, Efrat; Fischer, Bilha; Duval, Martine; D'Orleans-Juste, Pedro; Beaudoin, Adrien R.
CS Department de Biologie, Universite de Sherbrooke, Sherbrooke, QC, J1K 2R1, Can.
SO Journal of Medicinal Chemistry (2000), 43(11), 2239-2247
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB To elucidate the physiol. role played by **nucleoside triphosphate diphosphohydrolase** (**NTPDase**; EC 3.6.1.5), adenine nucleotide analogs, modified on the purine ring, have been synthesized and tested as potential inhibitors. Resistance of ATP analogs to hydrolysis and their potency as **NTPDase** inhibitors were evaluated. For this purpose, a particulate fraction isolated from bovine spleen was used as the enzyme source. Among the synthesized analogs, 8-thiobutyladenosine 5'-triphosphate (8-BuS-ATP) was found to be the most effective nonhydrolyzable competitive inhibitor, with an estimated Ki of 10 μM. This nonhydrolyzable analog did not exert any P2X-receptor-mediated effect on endothelium-denuded blood vessels, from the guinea pig mesenteric bed. In agreement with this observation, infusion of the analog did not cause any significant blood pressure variations of the precontracted vessel. Because in previous studies on isolated turkey erythrocytes and rat astrocytes 8-BuS-ATP was not able to trigger any P2Y1-receptor-mediated effect, it therefore appears that this **NTPDase** inhibitor does not interfere with purinergic receptors.
IT **284040-53-5 284040-54-6 284040-59-1 284040-60-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(synthesis and biochem. and pharmacol. characterizations of novel inhibitors of **nucleoside triphosphate diphosphohydrolases**)
RN 284040-53-5 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(hexylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



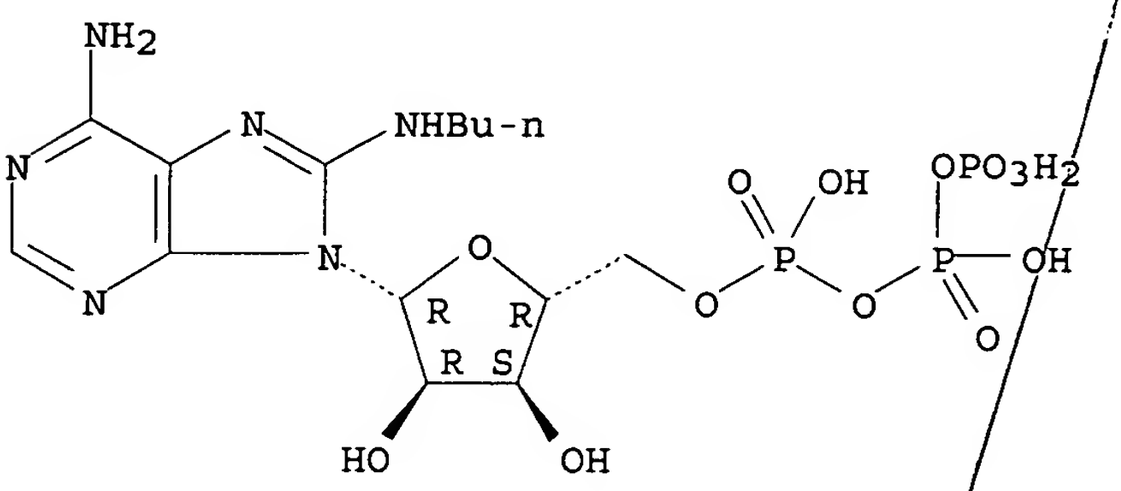
RN 284040-54-6 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



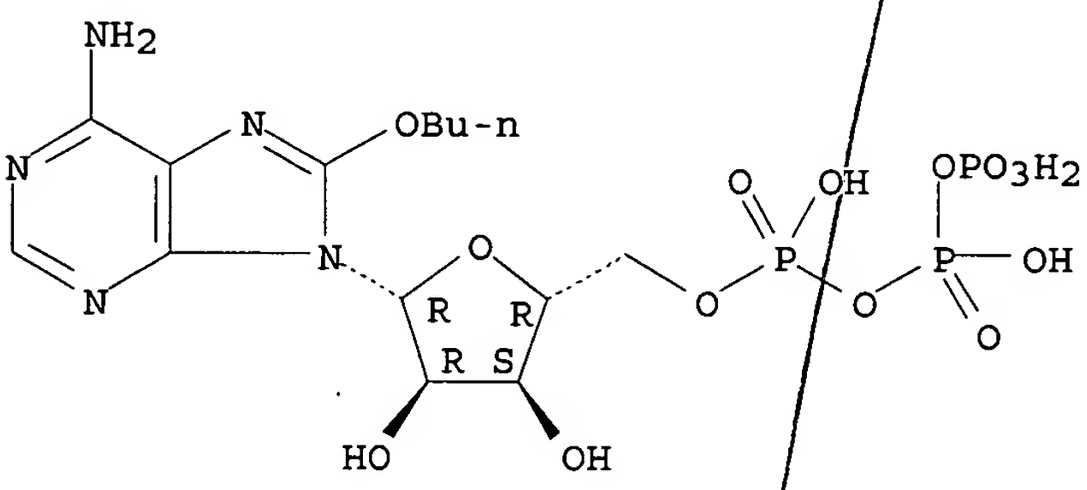
RN 284040-59-1 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylamino)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



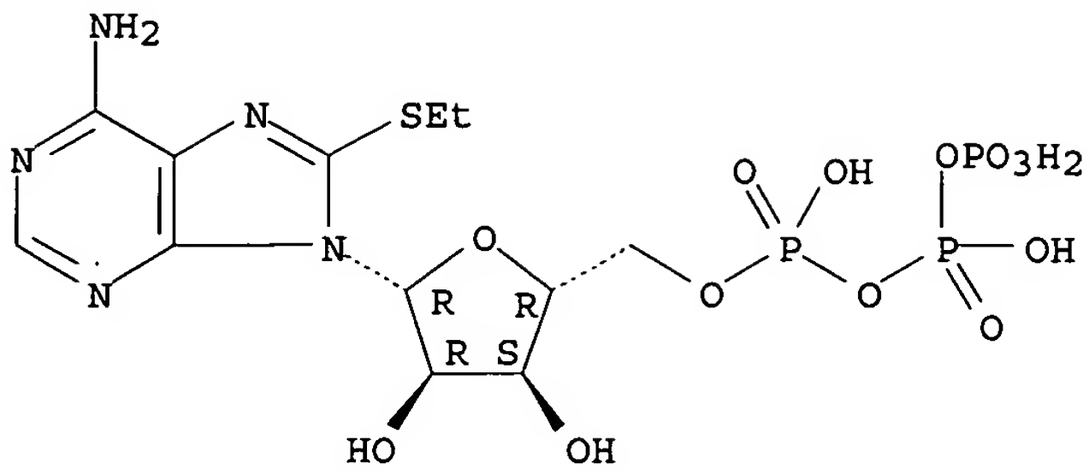
RN 284040-60-4 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-butoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



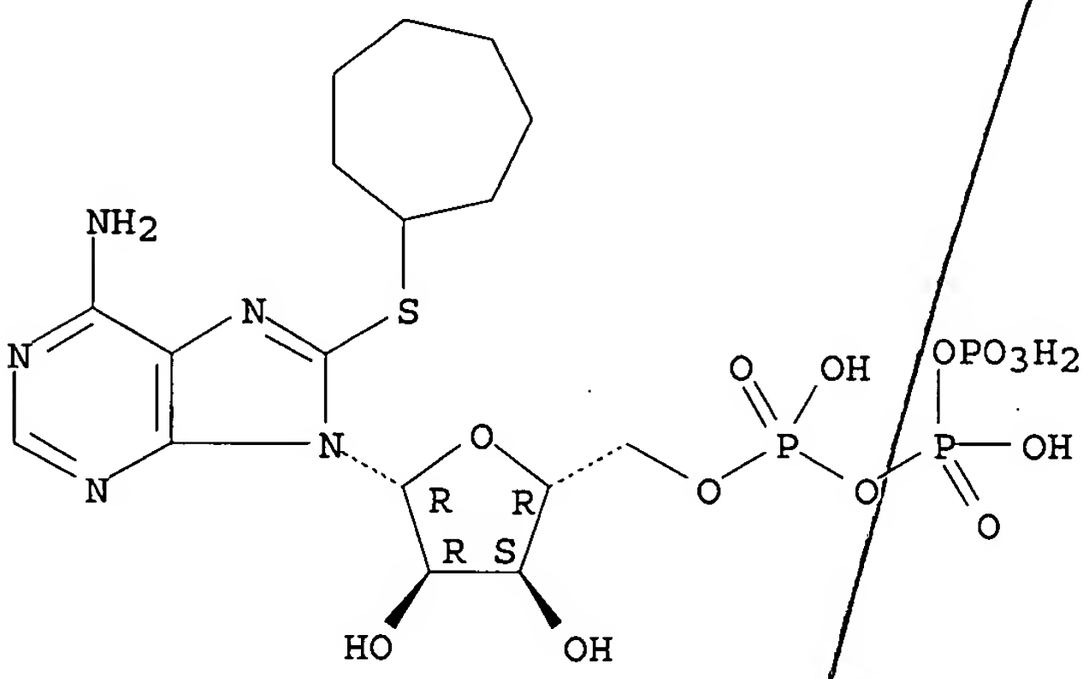
IT **81609-35-0P 284040-51-3P 284040-52-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biochem. and pharmacol. characterizations of novel inhibitors of **nucleoside triphosphate diphosphohydrolases**)
RN 81609-35-0 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(ethylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



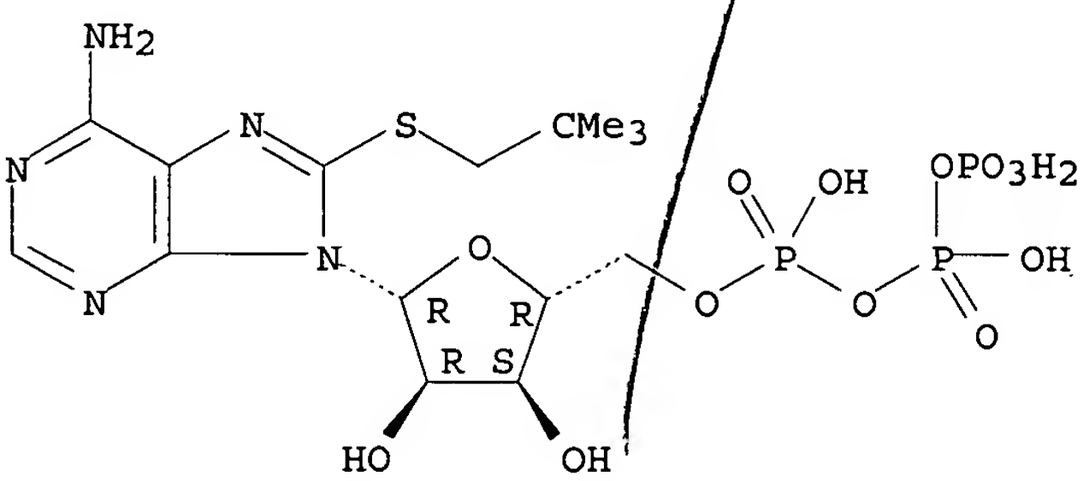
RN 284040-51-3 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(cycloheptylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 284040-52-4 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-[(2,2-dimethylpropyl)thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



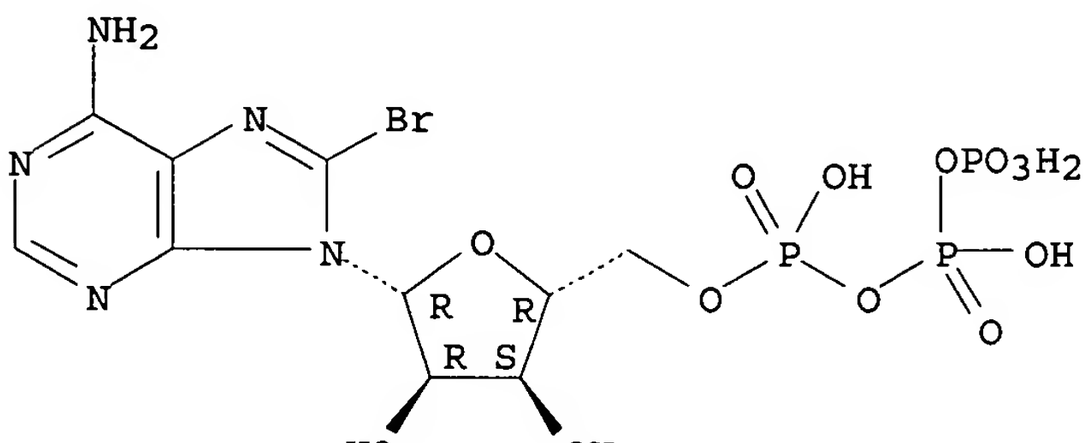
RE.CNT 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1997:285894 CAPLUS
DN 126:340339
TI Inhibition of **ecto-ATPase** by the P2 purinoceptor agonists, ATPγS, α,β-methylene-ATP, and AMP-PNP, in endothelial cells
AU Chen, Bing Chang; Lin, Wan-Wan
CS Department of Pharmacology, College of Medicine, National Taiwan University, Taipei, Taiwan
SO Biochemical and Biophysical Research Communications (1997), 233(2), 442-446

Printed

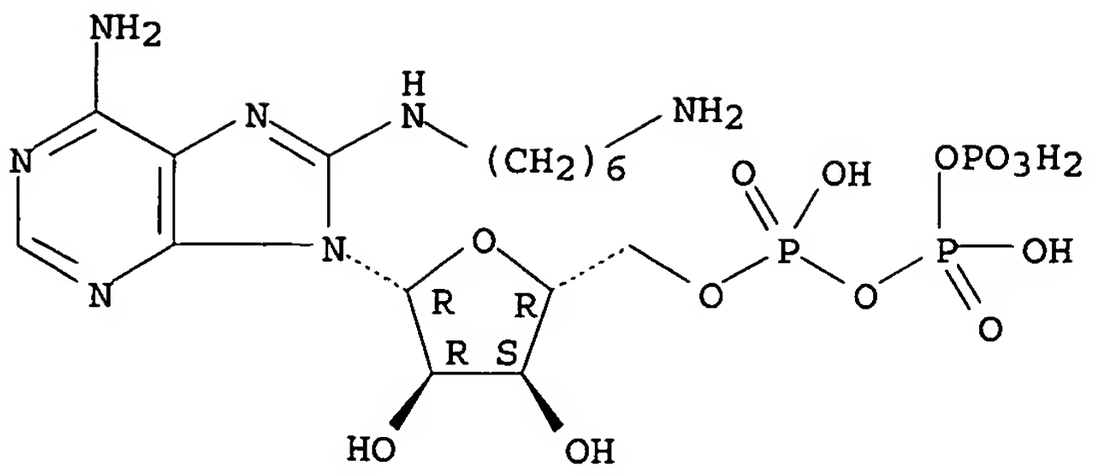
CODEN: BBRCA9; ISSN: 0006-291X
PB Academic
DT Journal
LA English
AB **Ecto-ATPase** is a plasma membrane-bound enzyme that sequentially dephosphorylates extracellular nucleotides such as ATP. This breakdown of ATP and other nucleotides makes it difficult to characterize and classify P2 purinoceptors. We have previously shown that the P2 purinergic antagonists, PPADS, suramin and reactive blue, act as **ecto-ATPase** inhibitors in various cell lines. Here, we show that the P2 purinergic agonists, ATPγS, α,β-methylene ATP (α,β-MeATP) and AMP-PNP, inhibit the **ecto-ATPase** of bovine pulmonary artery endothelial cells (CPAE), with pIC50 values of 5.2, 4.5 and 4.0, resp. In CPAE, FPL67156, a selective **ecto-ATPase** inhibitor, also inhibits **ecto-ATPase** activity, with a pIC50 value of 4.0. In addition, α,β-MeATP (3-100 μM), which itself does not induce phosphoinositide (PI) turnover, left-shifted the agonist-concentration effect (E/[A]) curves for ATP, 2MeS-ATP and UTP by approx. 100-300 fold, while those for ATPγS and AMP-PNP were only shifted approx. 2-3 fold. Moreover, in the presence of α,β-MeATP, not only was the potentiation effect of PPADS on the UTP response lost, but a slight inhibition of the UTP response by PPADS was also seen. Thus, we conclude that the action of ATPγS, α,β-MeATP and AMP-PNP as **ecto-ATPase** inhibitors account for their high agonist potency, and also provide information for the development of **ecto-ATPase** inhibitors of high selectivity and potency.
IT **23567-97-7**, 8-Bromo-ATP **53602-90-7**, 8-(6-Aminohexyl)amino-ATP
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(inhibition of **ecto-ATPase** by P2 purinoceptor agonists, ATPγS, α,β-methylene-ATP, and AMP-PNP, in endothelial cells)
RN 23567-97-7 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-bromo- (9CI). (CA INDEX NAME)

Absolute stereochemistry.



RN 53602-90-7 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-[(6-aminohexyl)amino]- (9CI) (CA INDEX NAME)

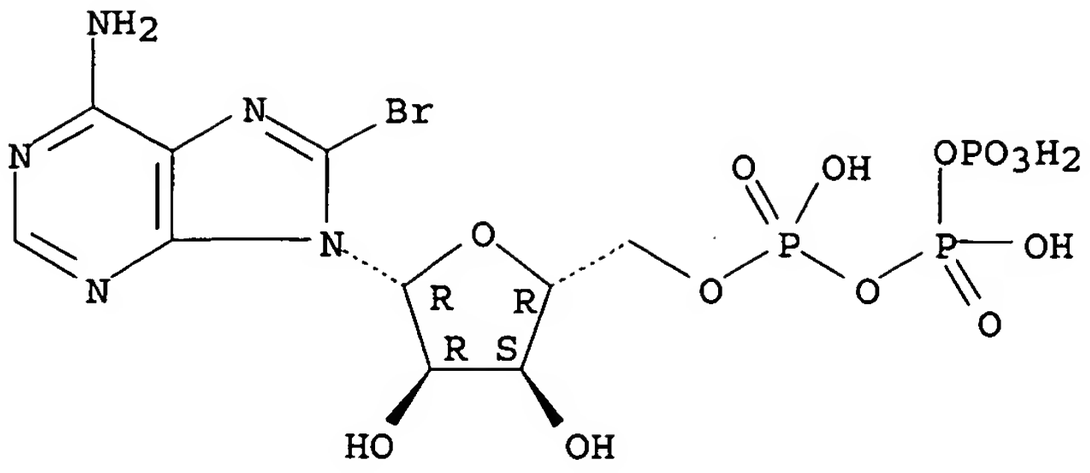
Absolute stereochemistry.



RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1996:300566 CAPLUS
DN 124:336420
TI Hydrolysis of P2-purinoceptor agonists by a purified **ectonucleotidase** from the bovine aorta, the ATP-diphosphohydrolase
AU Picher, Maryse; Sevigny, Jean; D'Orleans-Juste, Pedro; Beaudoin, Adrien R.
CS Fac. Sci., Univ. Sherbrooke, Sherbrooke, QC, Can.
SO Biochemical Pharmacology (1996), 51(11), 1453-1460
CODEN: BCPCA6; ISSN: 0006-2952
PB Elsevier
DT Journal
LA English
AB Pharmacologists are becoming more and more aware of the possibility that certain ATP analogs currently used to classify the P2-purinoceptors are dephosphorylated by **ectonucleotidases**. In this study, the authors provide evidence that in the vascular system, these purine analogs are hydrolyzed by an ATP-diphosphohydrolase (**ATPDase**). This enzyme is known as the major plasma membrane nucleotidase of endothelial and smooth muscle cells, and it believed to dephosphorylate extracellular triphospho- and diphosphonucleosides. Assays were conducted with a purified **ATPDase** from smooth muscle cells of bovine aorta. At a concentration of 250 μM, adenosine 5'-(α,β-methylene) triphosphonate (α,β-metATP), adenosine 5'-(β,γ-methylene) triphosphonate (β,γ-metATP), adenosine 5'-(α,β-methylene) diphosphonate (α,β-metADP), adenylyl 5'-(β,γ-imido) diphosphonate (β,γ-metATP), adenosine 5'-O-(2-thiodiphosphate) (ADPβS) all resisted dephosphorylation, whereas 2-chloroadenosine triphosphate (2-chloroATP), 2-methylthioadenosine triphosphate (2-MeSATP) and 8-bromoadenosine triphosphate (8-bromoATP) were hydrolyzed at 99, 63, and 20% of the rate of ATP hydrolysis, resp. All the non-hydrolyzable analogs tested, except α,β-metADP, competed with ATP and ADP for the **ATPDase** catalytic site, reducing their hydrolysis by 35-50%. Apparent Km values for ATP and ADP were estimated at 14.1 and 12.0 μM, resp., whereas apparent Km and Ki values for the purine analogs ranged from 12 to 28 μM. These results strongly support the view that (1) the **ATPDase** is expected to reduce substantially the P2-response induced by ATP, ADP, and some hydrolyzable agonists; and (2) by competing with the hydrolysis of endogenously released ATP and ADP, non-hydrolyzable analogs could alter the amplitude or direction of the cellular response induced by these natural substrates.
IT **23567-97-7**, 8-Bromoadenosine triphosphate
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(hydrolysis of P2-purinoceptor agonists by ATP-diphosphohydrolase from bovine aorta)
RN 23567-97-7 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-bromo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

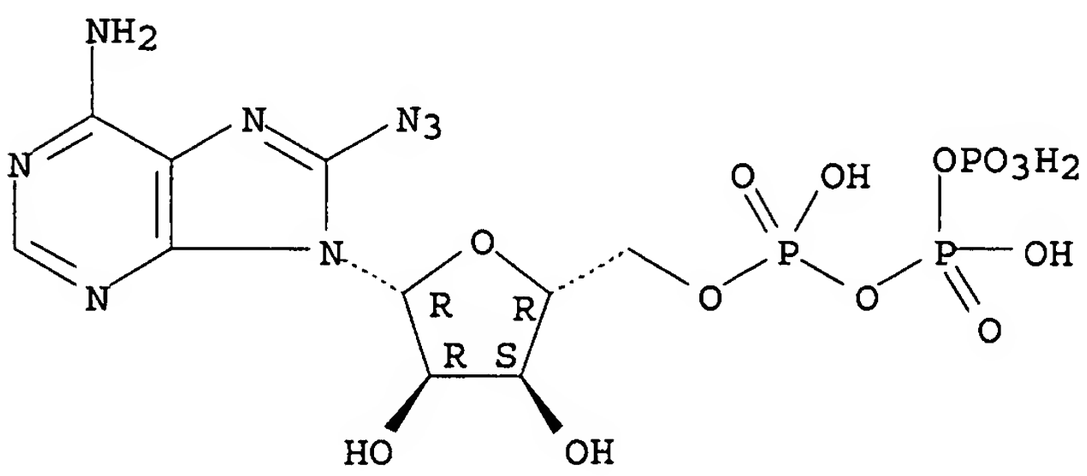


L11 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1994:50794 CAPLUS
DN 120:50794
TI 8-Azido-adenine nucleotides as substrates of ecto-nucleotidases in chromaffin cells: Inhibitory effect of photoactivation
AU Rodriguez-Pascual, Fernando; Torres, Magdalena; Miras-Portugal, M. Teresa
CS Fac. Vet., Univ. Complutense Madrid, Madrid, Spain
SO Archives of Biochemistry and Biophysics (1993), 306(2), 420-6
CODEN: ABBIA4; ISSN: 0003-9861
DT Journal
LA English

already printed article w/ N-linked cpds

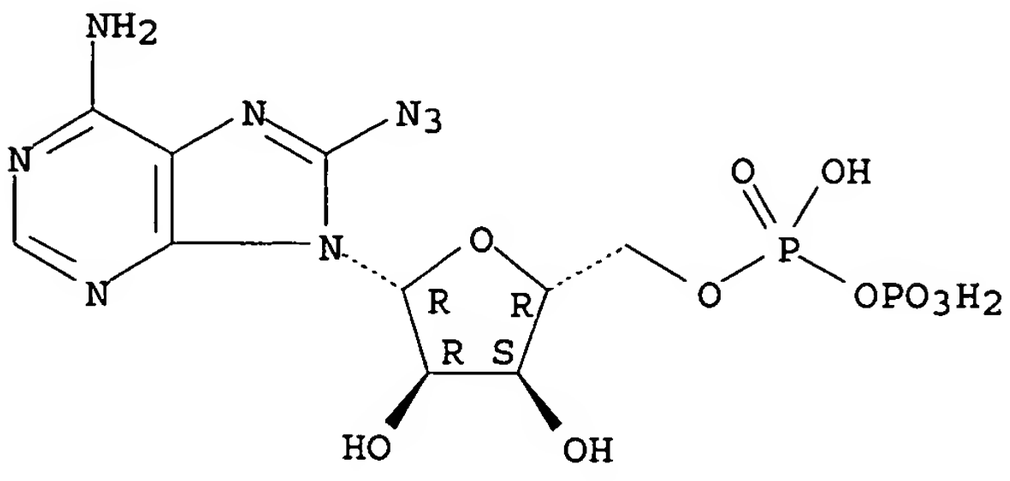
AB The components of the ecto-nucleotidase pathway at the extracellular surface of adrenal chromaffin cells are the enzymic activities responsible for the hydrolysis of granular nucleotide compds. released during the secretory response. The azido-nucleotides have been largely employed to characterize nucleotide binding sites. The 8-azido-adenine nucleotides were studied as substrates of ecto-nucleotidases in cultured chromaffin cells by HPLC procedures. 8-Azido-ATP (8-N3-ATP) was a good substrate for **ecto-ATPase** activity, the Km value was 256.30 ± 36.41 μM, and the Vmax value was 14.33 ± 0.84 nmol/min + 106 cells. 8-Azido-ADP (8-N3-ADP) was dephosphorylated by the ecto-ADPase activity with a Km value of 595.29 ± 67.44 μM and Vmax value of 6.86 ± 0.45 nmol/min + 106 cells. These kinetic parameters were similar to those obtained with ATP and ADP in the same culture and incubation conditions. 8-Azido-AMP (8-N3-AMP) was not hydrolyzed by the ecto-5'-nucleotidase activity. The 8-azido-nucleotides competitively inhibited the hydrolysis of adenine nucleotides, with Ki values in the same range as the Km. After UV photoactivation, the three 8-azido-nucleotides (100 μM) irreversibly inhibited and to a similar extent, between 40 and 55%, each of ecto-nucleotidase activities. UV photoactivation in the presence of nucleotides in the same concentration range was an effective protection from the inhibition.
IT **53696-59-6**, 8-Azido-ATP **59432-65-4**, 8-Azido-ADP
60731-47-7, 8-Azido-AMP
RL: BIOL (Biological study)
(ecto-nucleotidase specificity for, in adrenal medulla chromaffin cell, photoactivation study of)
RN 53696-59-6 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-azido- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



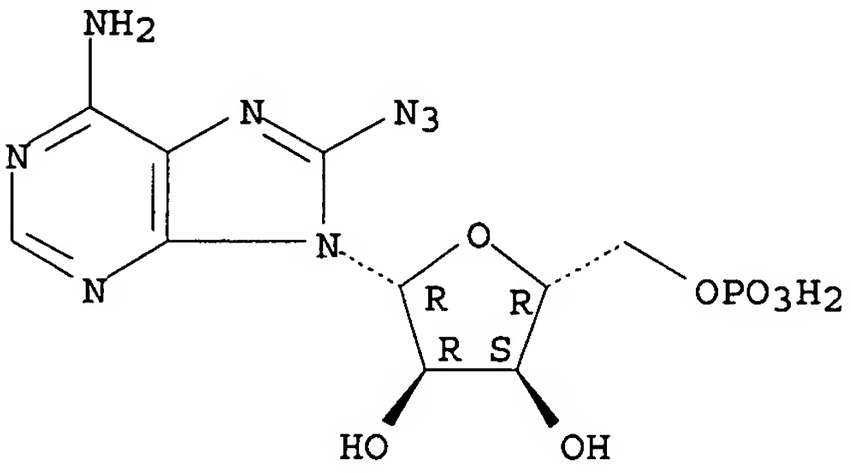
RN 59432-65-4 CAPLUS
CN Adenosine 5'-(trihydrogen diphosphate), 8-azido- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 60731-47-7 CAPLUS
CN 5'-Adenylic acid, 8-azido- (9CI) (CA INDEX NAME)

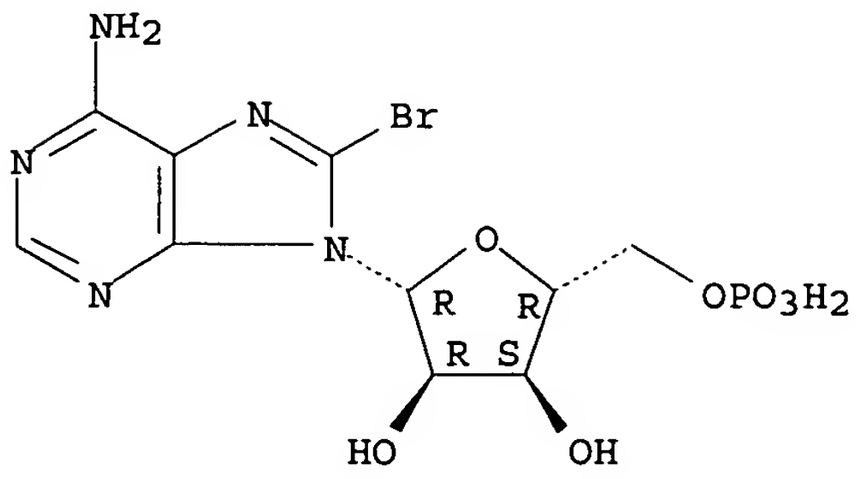
Absolute stereochemistry.



L11 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1987:590370 CAPLUS
DN 107:190370
TI The structure-activity relationships of **ectonucleotidases** and of excitatory P2-purinoceptors: evidence that dephosphorylation of ATP analogs reduces pharmacological potency
AU Welford, Laurence A.; Cusack, Noel J.; Hourani, Susanna M. O.
CS King's Coll., Univ. London, London, WC2R 2LS, UK
SO European Journal of Pharmacology (1987), 141(1), 123-30
CODEN: EJPHAZ; ISSN: 0014-2999
DT Journal
LA English
AB The dephosphorylation of adenine nucleotides and their analogs by **ectonucleotidases** on the guinea pig urinary bladder was studied using HPLC. The rate of dephosphorylation of each analog was compared with its pharmacol. potency at causing contraction. ATP, ADP, and AMP were rapidly dephosphorylated, and substitution on the purine ring did not affect the rate of breakdown. The **ectonucleotidases** showed stereoselectivity towards the ribose moiety and towards the polyphosphate chain. In general, methylene isosteres of the nucleotides, and analogs in which 1 of the O atoms on the terminal phosphate had been replaced, were resistant to degradation None of the analogs that were readily dephosphorylated was more potent than ATP, and most, but not all, of the analogs resistant to degradation were more potent than ATP, suggesting that although resistance to degradation does not in itself confer high potency, susceptibility to degradation does limit the potency of ATP and its degradable analogs.
IT **23567-96-6 23567-97-7 23600-16-0**, 8-Bromo-ADP
RL: BIOL (Biological study)
(bladder contraction by, structure in relation to)
RN 23567-96-6 CAPLUS
CN 5'-Adenylic acid, 8-bromo- (9CI) (CA INDEX NAME)

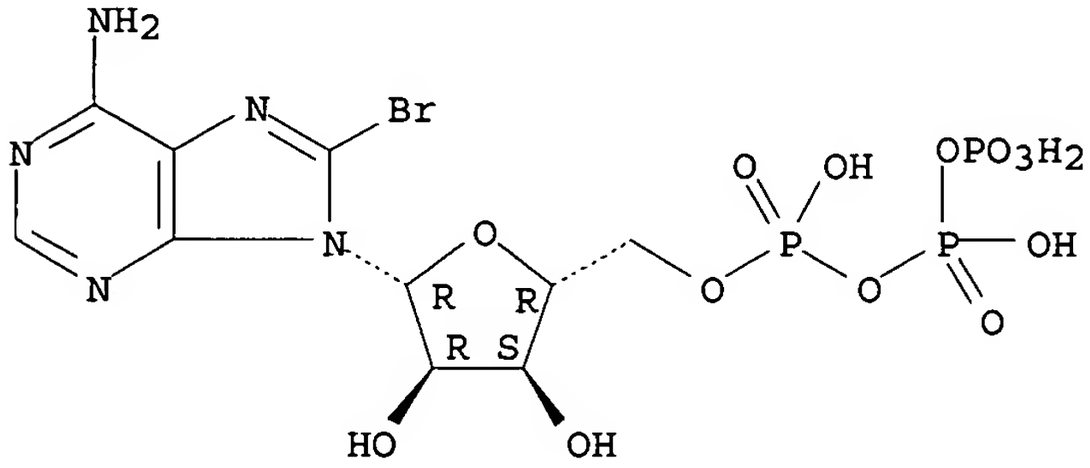
already printed article of these cpds.

Absolute stereochemistry.



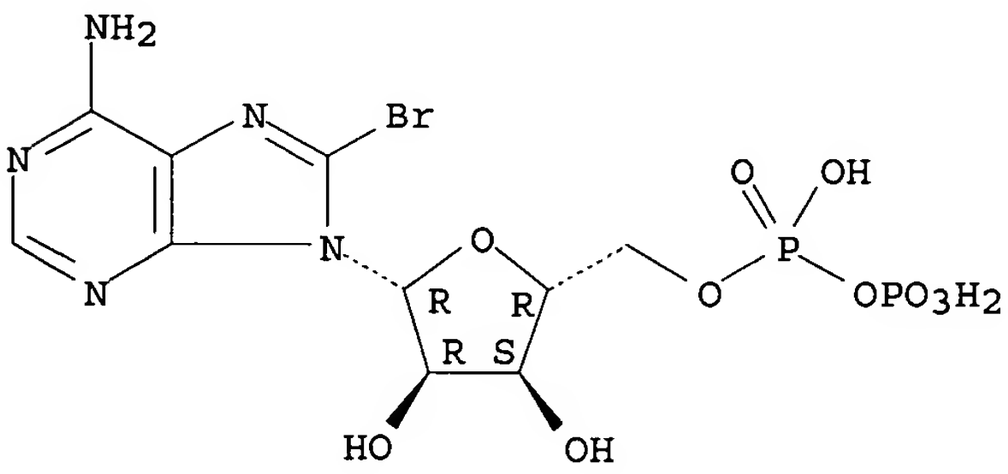
RN 23567-97-7 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-bromo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 23600-16-0 CAPLUS
CN Adenosine 5'-(trihydrogen diphosphate), 8-bromo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L11 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1987:12328 CAPLUS
DN 106:12328
TI ATP analogs and the guinea pig tenia coli: a comparison of the structure-activity relationships of **ectonucleotidases** with those of the P2-purinoceptor
AU Welford, Laurence A.; Cusack, Noel J.; Hourani, Susanna M. O.
CS King's Coll., Univ. London, London, WC2R 2LS, UK
SO European Journal of Pharmacology (1986), 129(3), 217-24
CODEN: EJPHAZ; ISSN: 0014-2999
DT Journal
LA English
AB The dephosphorylation of adenine nucleotides and their analogs by **ectonucleotidase** [9027-73-0] in the guinea pig tenia coli was studied using HPLC. The rate of dephosphorylation of each analog was compared with its pharmacol. potency relative to ATP [56-65-5]. ATP, ADP

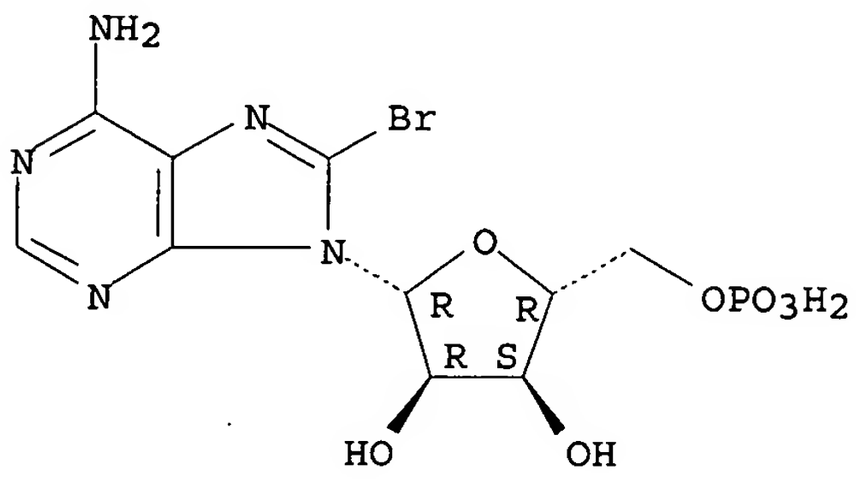
already printed article of these cpds.

[58-64-0] and AMP [61-19-8] were rapidly dephosphorylated, and substitution on the purine ring had no effect upon the rate of breakdown. The **ectonucleotidases** showed stereoselectivity towards the ribose, the unnatural L-enantiomers of nucleotides being dephosphorylated more slowly. Analogs in which one of the O atoms on the terminal phosphate had been replaced were resistant to degradation Phosphorothioate analogs in which a sulfur was attached to the penultimate phosphorus were degraded stereoselectively. Methylene isosteres of ATP and ADP resisted degradation, except for homo-ATP [72041-44-2] which was dephosphorylated at the same rate as ATP. Overall, no correlation was found between the potency of an analog and its rate of degradation

IT **23567-96-6**, 8-Bromoadenosine 5'-monophosphate **23567-97-7**, 8-Bromoadenosine 5'-triphosphate **23600-16-0**, 8-Bromoadenosine 5'-diphosphate
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(metabolism of, by **ectonucleotidase** of tenia coli, P2-purinergic agonist activity in relation to)

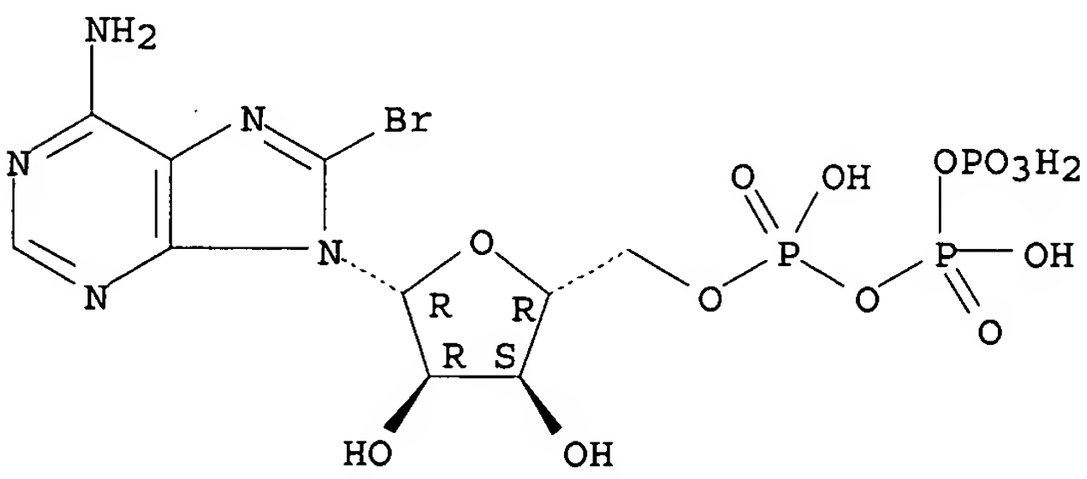
RN 23567-96-6 CAPLUS
CN 5'-Adenylic acid, 8-bromo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



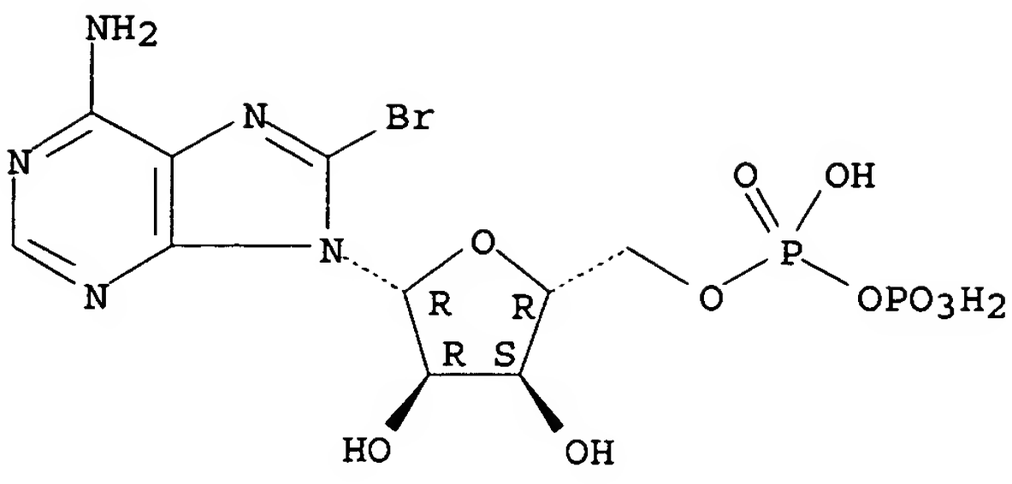
RN 23567-97-7 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-bromo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 23600-16-0 CAPLUS
CN Adenosine 5'-(trihydrogen diphosphate), 8-bromo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.


NH2
N
Br
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NEWS 16	MAY 10	CA/CAplus enhanced with 1900-1906 U.S. patent records
NEWS 17	MAY 11	KOREAPAT updates resume
NEWS 18	MAY 19	Derwent World Patents Index to be reloaded and enhanced

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FULL SEARCH INITIATED 00:34:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 73256 TO ITERATE

100.0% PROCESSED 73256 ITERATIONS 1324 ANSWERS

SEARCH TIME: 00.00.01

L2 1324 SEA SSS FUL L1

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COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
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FILE LAST UPDATED: 25 May 2006 (20060525/ED)

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103702 AGGREGATION
2116 AGGREGATIONS
L3 105070 AGGREGATION
(AGGREGATION OR AGGREGATIONS)

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L4 2 THROMBOGENECITY

=> s thrombogenec?
L5 2 THROMBOGENEC?

=> s thrombogenec
=> s l2
L6 1225 L2

=> s l6 and (l3 or l4 or l5)
L7 14 L6 AND (L3 OR L4 OR L5)

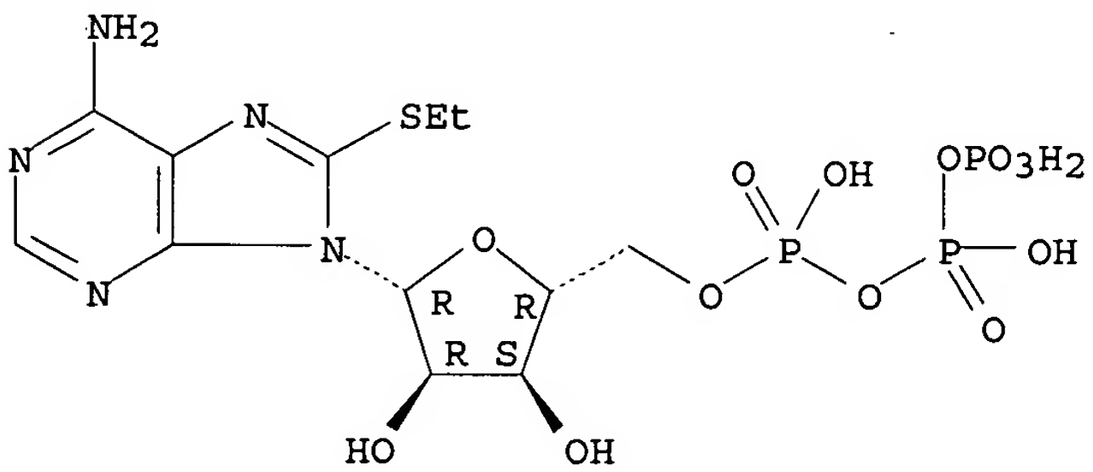
=> d bib abs hitstr 1-14 l7

L7 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:911398 CAPLUS
DN 142:214281
TI C8-substituted purine nucleotide analogs and their use as inhibitors of nucleoside triphosphate diphosphohydrolases
IN Halbfinger, Efrat; Fischer, Bilha; Beaudoin, Adrien R.; Gendron, Fernand Pierre
PA Universite de Sherbrooke, Can.; Bar-Ilan University
SO Can. Pat. Appl., 54 pp.
CODEN: CPXXEB
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

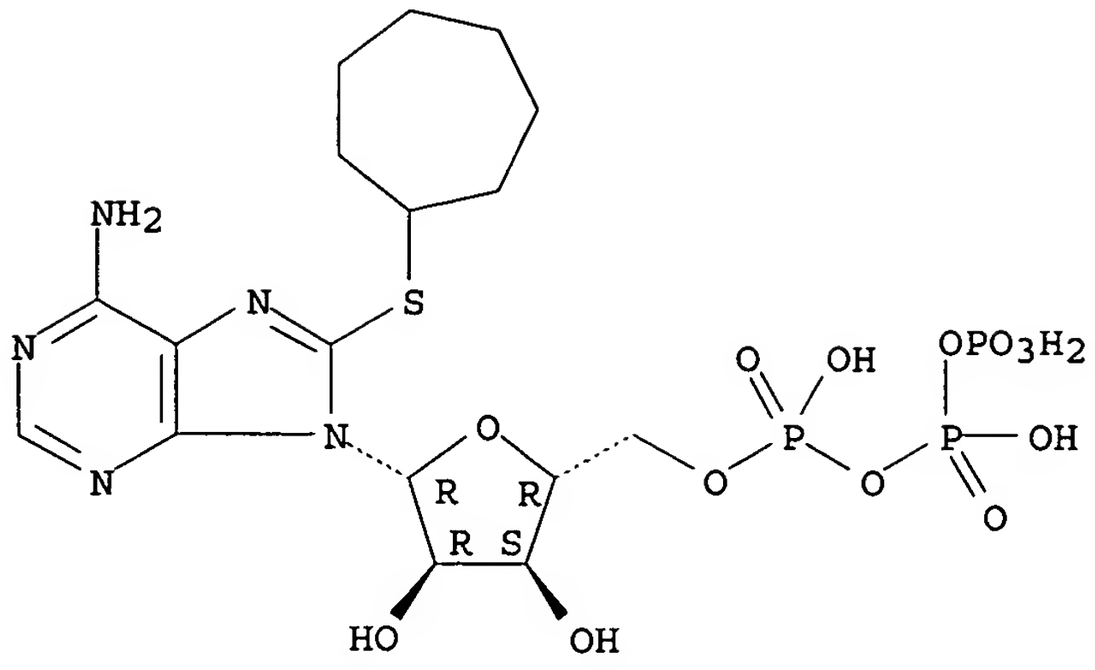
PI CA 2311084 AA 20011209 CA 2000-2311084 20000609
PRAI CA 2000-2311084 20000609
OS CASREACT 142:214281
AB Ectonucleoside triphosphate diphosphohydrolases [NTPDases; EC 3.6.1.5] constitute a family of enzymes which are involved in the metabolism of extracellular nucleotides, catalyzing the hydrolysis of the gamma and beta phosphate bonds of triphospho- and diphosphonucleosides (whereas 5'-nucleotidases [EC 3.1.3.5] catalyze the hydrolysis of alpha phosphate bond of monophosphonucleosides). These extracellular nucleotides interact with endothelial, epithelial and smooth muscle cells, as well as blood cells and lymphoid cells, to influence the different physiol. systems of vertebrates. Since these ecto-nucleotidases alter the extracellular concns. of nucleotides these enzymes modulate their physiol. effects, including, for example, platelet **aggregation**, heart function, control of vascular tone and inflammation reactions, electrolyte secretion and gastrointestinal motility, neurotransmission both in central and peripheral nervous systems, as well as other effects in other physiol. systems. This invention provides C8 substituted purine nucleotide analogs, such as ATP analogs, and further provides their use as inhibitors of NTPDases and thereby as tools to modulate the conversion of nucleotides into nucleoside derivs., and thus modulate the levels of these compds. Such modulation further provides for the modulation of the activity and function of many processes which are affected by these compds.
IT **81609-35-0P 284040-51-3P 284040-52-4P 284040-53-5P**
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(C8-substituted purine nucleotide analogs and their use as inhibitors of nucleoside triphosphate diphosphohydrolases to modulate purine nucleotide levels and biol. processes)
RN 81609-35-0 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(ethylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



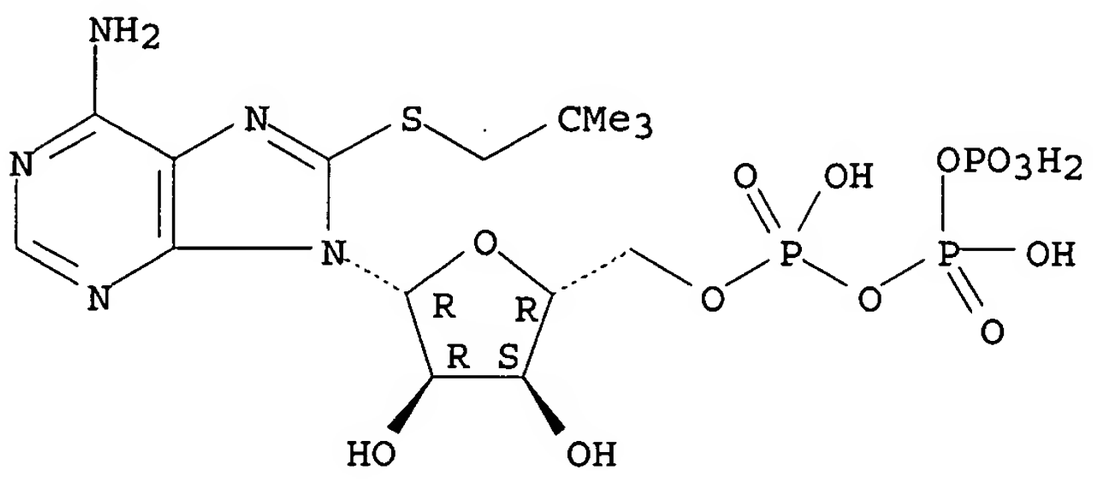
RN 284040-51-3 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(cycloheptylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



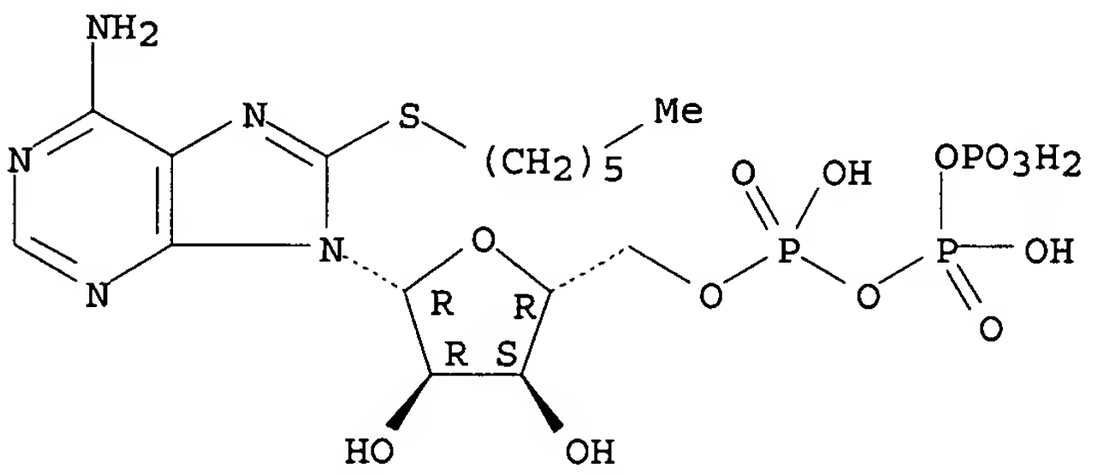
RN 284040-52-4 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-[(2,2-dimethylpropyl)thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



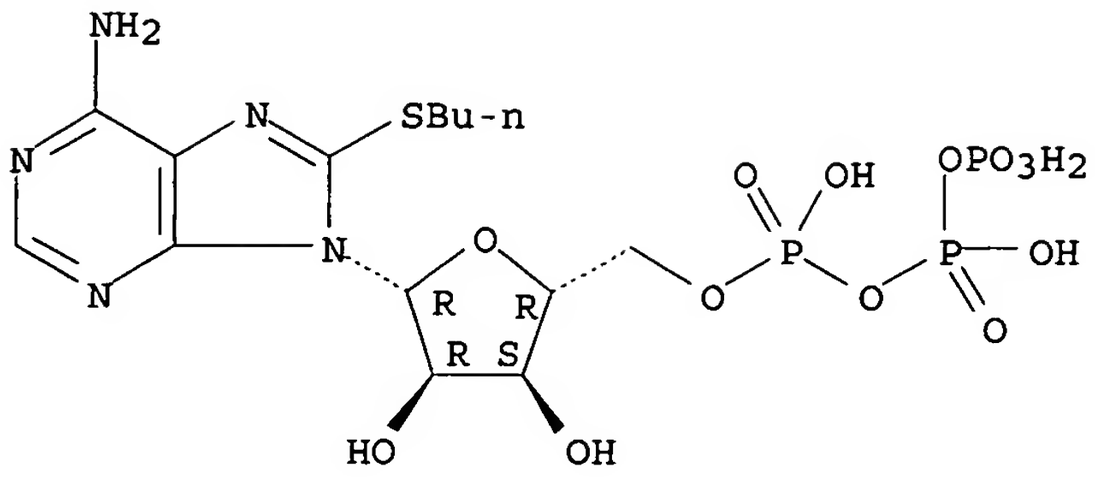
RN 284040-53-5 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(hexylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



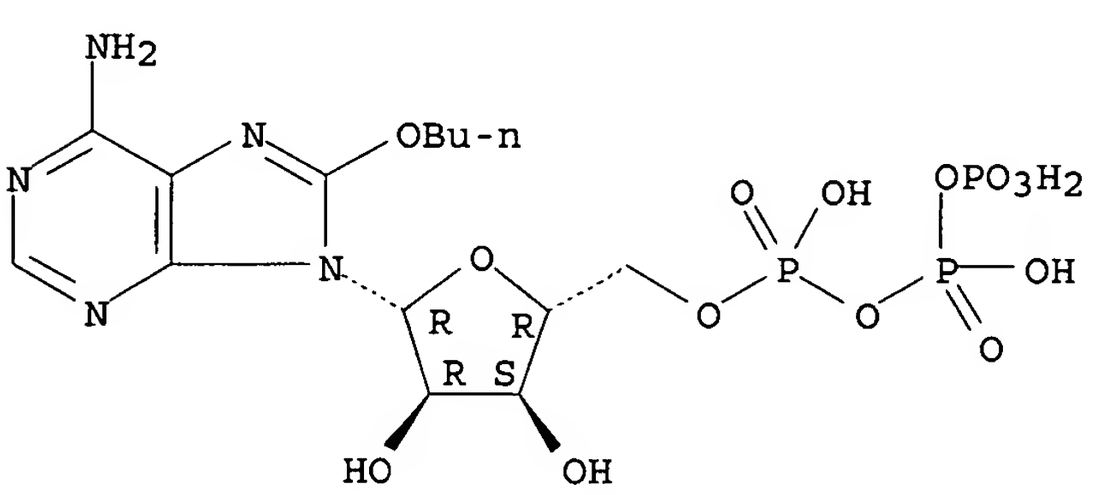
IT **284040-54-6 284040-60-4**
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(C8-substituted purine nucleotide analogs and their use as inhibitors of nucleoside triphosphate diphosphohydrolases to modulate purine nucleotide levels and biol. processes)
RN 284040-54-6 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



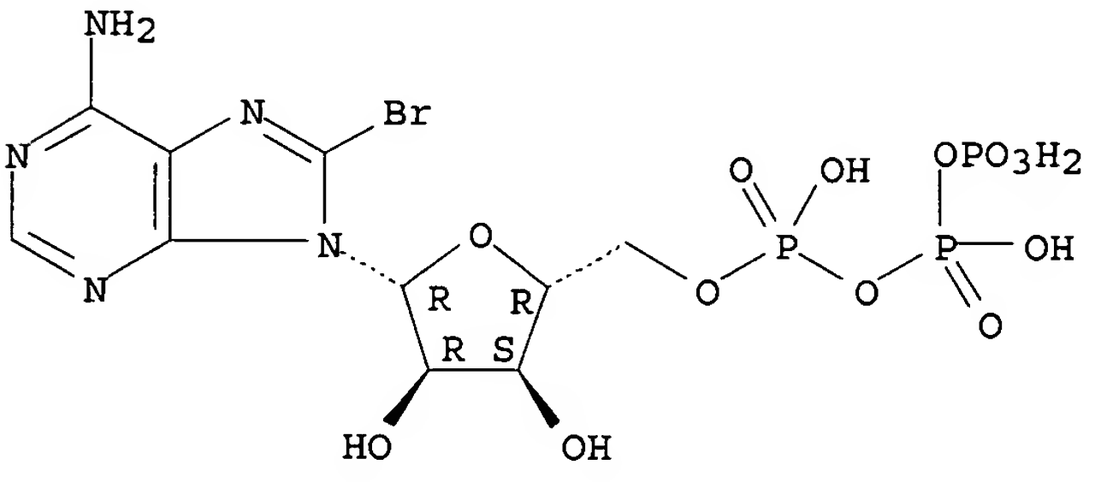
RN 284040-60-4 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-butoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



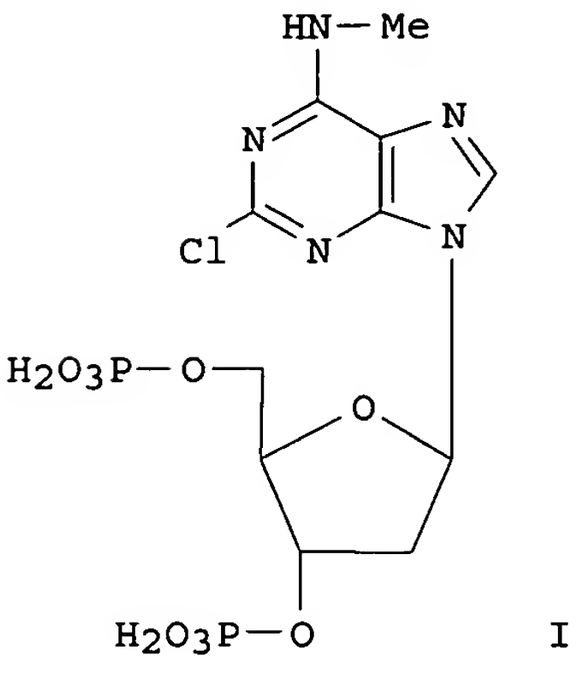
IT **23567-97-7**, 8-Bromo-ATP
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(substrate; C8-substituted purine nucleotide analogs and their use as inhibitors of nucleoside triphosphate diphosphohydrolases to modulate purine nucleotide levels and biol. processes)
RN 23567-97-7 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-bromo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1999:245290 CAPLUS
DN 131:59076
TI Structure-Activity Relationships of Bisphosphate Nucleotide Derivatives as P2Y1 Receptor Antagonists and Partial Agonists
AU Nandanan, Erathodiyil; Camaioni, Emidio; Jang, Soo-Yeon; Kim, Yong-Chul; Cristalli, Gloria; Herdewijn, Piet; Secrist, John A., III; Tiwari, Kamal N.; Mohanram, Arvind; Harden, T. Kendall; Boyer, Jose L.; Jacobson, Kenneth A.
CS Molecular Recognition Section Laboratory of Bioorganic Chemistry, National Institute of Diabetes Digestive and Kidney Diseases, National Institutes of Health, Bethesda, MD, 20892-0810, USA
SO Journal of Medicinal Chemistry (1999), 42(9), 1625-1638

CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
GI



I

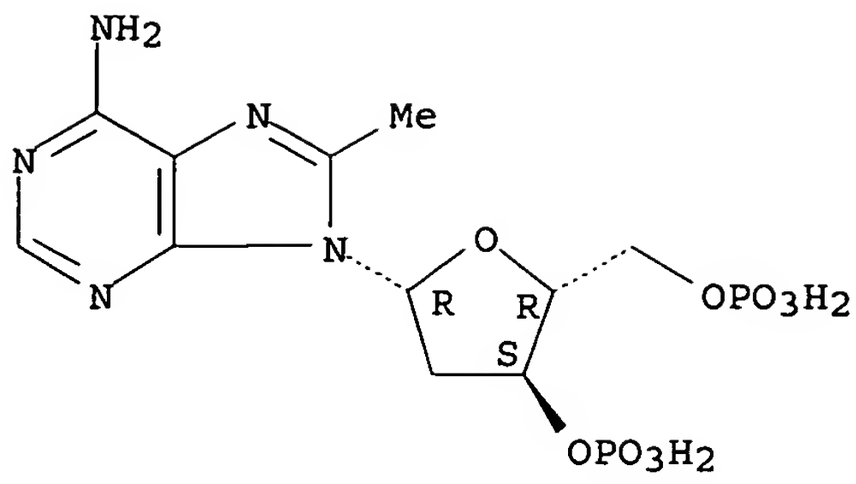
AB The P2Y1 receptor is present in the heart, in skeletal and various smooth muscles, and in platelets, where its activation is linked to **aggregation**. Adenosine 3',5'- and 2',5'-bis-phosphates have been identified as selective antagonists at the P2Y1 receptor and have been modified structurally to increase receptor affinity. We have extended the structure-activity relationships to a new series of deoxyadenosine bis-phosphates with substitutions in the adenine base, ribose moiety, and phosphate groups. The activity of each analog at P2Y1 receptors was determined by measuring its capacity to stimulate phospholipase C in turkey erythrocyte membranes (agonist effect) and to inhibit phospholipase C stimulation elicited by 10 nM 2-(methylthio)ADP (antagonist effect). 2'-Deoxyadenosine bis-phosphate analogs containing halo, amino, and thioether groups at the 2-position of the adenine ring were more potent P2Y1 receptor antagonists than analogs containing various heteroatom substitutions at the 8-position. An N6-methyl-2-chloro analog I, was a full antagonist and displayed an IC50 of 206 nM. On the ribose moiety, 2'-hydroxy, 4'-thio, carbocyclic, and six-membered anhydro-hexitol ring modifications have been prepared and resulted in enhanced agonist properties. The 1,5-anhydro-hexitol analog was a pure agonist with an EC50 of 3 μM, i.e., similar in potency to ATP 5'-Phosphate groups have been modified in the form of triphosphate, Me phosphate, and cyclic 3',5'-diphosphate derivs. The carbocyclic analog had enhanced agonist efficacy, and the 5'-O-phosphonyl-Me modification was tolerated, suggesting that deviations from the nucleotide structure may result in improved utility as pharmacol. probes. The N6-methoxy modification eliminated receptor affinity. Pyrimidine nucleoside 3',5'-bis-phosphate derivs. were inactive as agonists or antagonists at P2Y receptor subtypes.

IT **228264-34-4P 228264-35-5P 228264-36-6P**
228264-37-7P 228264-38-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and structure-activity relationships of bis-phosphate nucleotides as P2Y1 receptor antagonists and partial agonists)

RN 228264-34-4 CAPLUS

CN 3'-Adenylic acid, 2'-deoxy-8-methyl-, 5'-(dihydrogen phosphate), ammonium salt (9CI) (CA INDEX NAME)

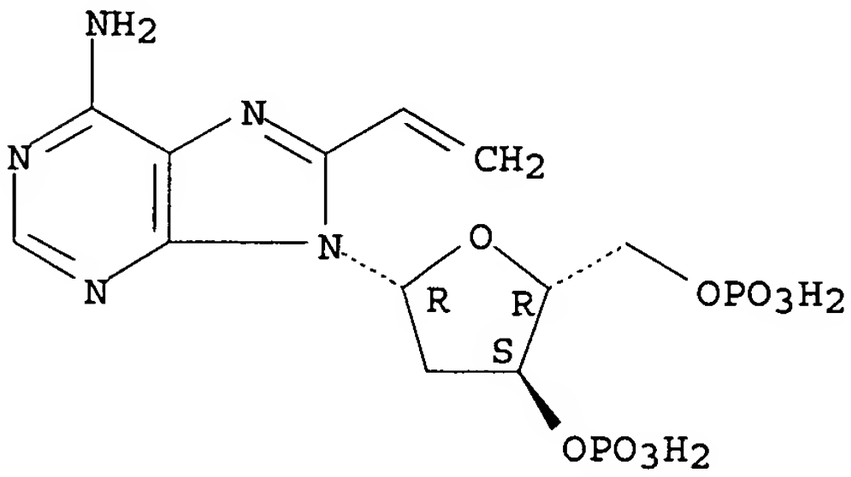
Absolute stereochemistry.



●x NH3

RN 228264-35-5 CAPLUS
CN 3'-Adenylic acid, 2'-deoxy-8-ethenyl-, 5'-(dihydrogen phosphate), ammonium salt (9CI) (CA INDEX NAME)

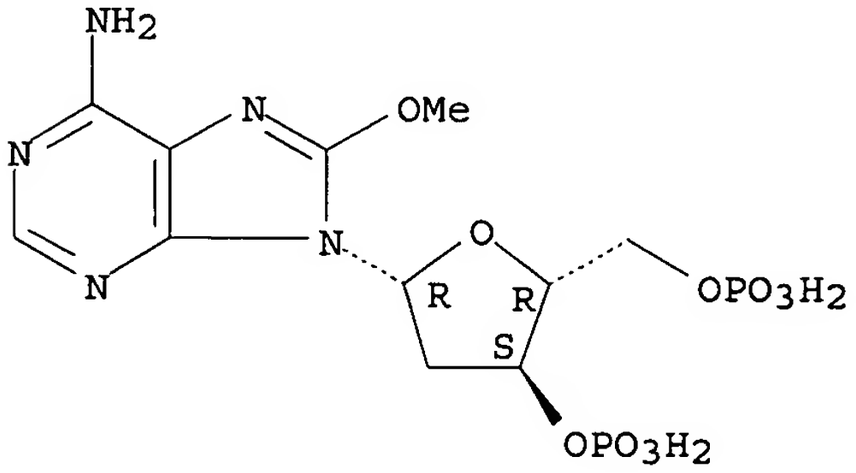
Absolute stereochemistry.



●x NH3

RN 228264-36-6 CAPLUS
CN 3'-Adenylic acid, 2'-deoxy-8-methoxy-, 5'-(dihydrogen phosphate), ammonium salt (9CI) (CA INDEX NAME)

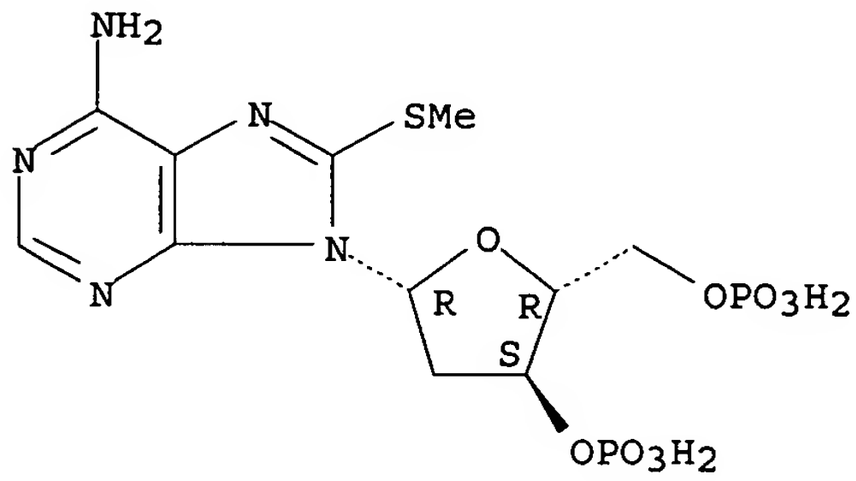
Absolute stereochemistry.



●x NH3

RN 228264-37-7 CAPLUS
CN 3'-Adenylic acid, 2'-deoxy-8-(methylthio)-, 5'-(dihydrogen phosphate), ammonium salt (9CI) (CA INDEX NAME)

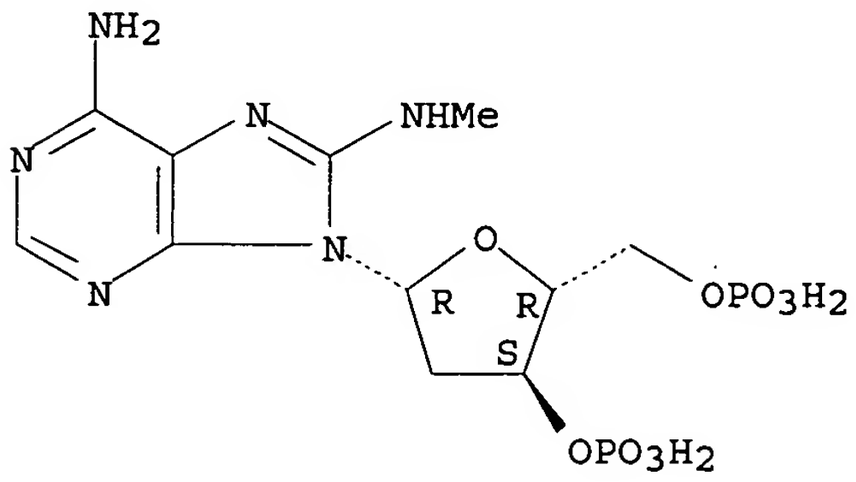
Absolute stereochemistry.



●x NH3

RN 228264-38-8 CAPLUS
CN 3'-Adenylic acid, 2'-deoxy-8-(methylamino)-, 5'-(dihydrogen phosphate), ammonium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●x NH3

RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1996:197574 CAPLUS
DN 124:313309
TI Platelet activation by 2-(4-bromo-2,3-dioxobutylthio)adenosine 5'-diphosphate is mediated by its binding to a putative ADP receptor, aggregin
AU Puri, Rajinder N.; Colman, Roberta F.; Colman, Robert W.
CS Sol Sherry Thrombosis Research Center, Temple Univ. School Medicine, Philadelphia, PA, USA
SO European Journal of Biochemistry (1996), 236(3), 862-70
CODEN: EJBCAI; ISSN: 0014-2956
PB Springer
DT Journal
LA English
AB Platelet responses induced by ADP are mediated by a unique P2T-purinergic receptor. Although a variety of ADP analogs, substituted at C2, were used to delineate pharmacol. properties of the ADP-binding site(s), the identity of the receptor protein was not firmly established. 2-(4-Bromo-2,3-dioxobutylthio)-ADP[2-BrCH2(CO)2CH2-S-ADP], a well-characterized ADP analog, was used as an affinity label to examine the structure/function relationship of ADP-requiring enzymes. It induced platelet shape change, **aggregation**, exposure of fibrinogen binding sites, secretion, and mobilization of intracellular Ca, but was less potent than ADP. Under non-stirring conditions, incubation of platelets with this analog for longer time periods blocked ADP-induced shape change, **aggregation**, and the ability of ADP to antagonize

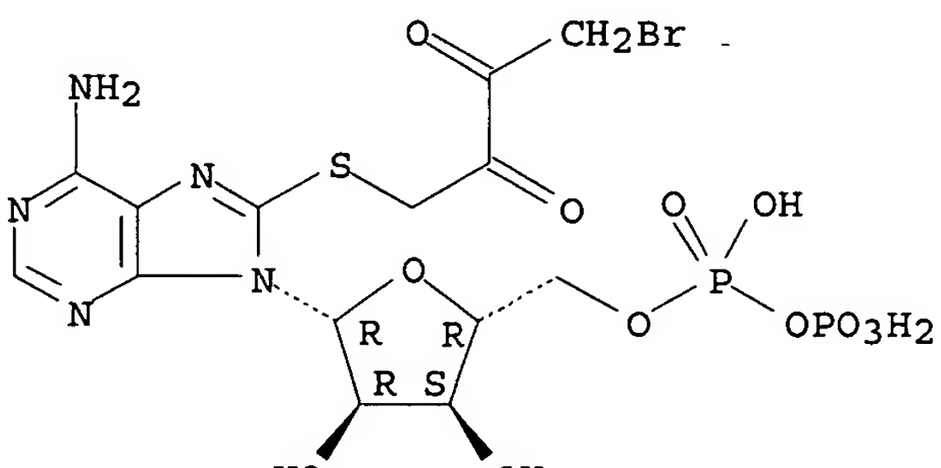
the rise in intracellular levels of cAMP induced by iloprost (a prostaglandin I2 analog). Of a variety of agonists examined, only ADP-induced **aggregation** was almost completely inhibited in platelets irreversibly modified by the analog. An autoradiogram of the gel obtained by SDS/PAGE of solubilized platelets modified by the ADP analog followed by reduction of the dioxo group by NaB[3H]4 showed the presence of a single radiolabeled protein band at 100 kDa. Platelets incubated 1st with either ADP, ATP, or 2-methylthio-ADP were not labeled by 2-BrCH2(CO)2CH2S-ADP and NaB[3H]4. 8-BrCH2(CO)2CH-S-ADP was previously shown by us to irreversibly antagonize ADP-induced platelet responses by selectively modifying aggregin. Incubation of platelets with 2-BrCH2(CO)2CH2S-ADP completely blocked labeling of aggregin in platelets by 8-BrCH2(CO)2CH2S-[32P]ADP. These results show that 2-BrCH2(CO)2CH2S-ADP initially interacts reversibly with aggregin (100 kDa), a putative ADP receptor, and induces platelet shape change and **aggregation**, and at longer periods of incubation reacts irreversibly to block the ability of ADP to antagonize stimulated adenylate cyclase activity. In contrast, 6-BrCH2(CO)2CH2S-ADP was found to be a weak and reversible inhibitor of ADP-induced platelet **aggregation**. Prior incubation of platelets with the latter analog reduced labeling of aggregin by 8-BrCH2(CO)2CH2S-[32P]ADP. Taken together, the results further show that substitution by the BrCH2(CO)2CH2 group at the C2 and C8 positions is tolerated, while the presence of a free amino function at the C6 position is essential for its interaction with aggregin.

IT **115678-78-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PNU (Preparation, unclassified); BIOL (Biological study); PREP (Preparation)
(platelet activation by 2-(4-bromo-2,3-dioxobutylthio)ADP is mediated by its binding to a putative ADP receptor, aggregin)

RN 115678-78-9 CAPLUS

CN Adenosine 5'-(trihydrogen diphosphate), 8-[(4-bromo-2,3-dioxobutyl)thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1995:880408 CAPLUS

DN 123:311093

TI Inhibition of ADP-induced platelet responses by covalent modification of aggregin, a putative ADP receptor, by 8-(4-bromo-2,3-dioxobutylthio)ADP

AU Puri, Rajinder N.; Kumar, Ajay; Chen, Haiying; Colman, Roberta F.; Colman, Robert W.

CS Sol Sherry Thrombosis Res. Cent., Temple Univ. Sch. Med., Philadelphia, PA, 19140, USA

SO Journal of Biological Chemistry (1995), 270(41), 24482-8
CODEN: JBCHA3; ISSN: 0021-9258

PB American Society for Biochemistry and Molecular Bio logy

DT Journal

LA English

AB ADP is an important platelet agonist which initiates platelet shape change, **aggregation**, exposure of fibrinogen receptors, and calcium mobilization. Because of the limitations of previously used affinity analogs and photolabeling studies as well as controversies

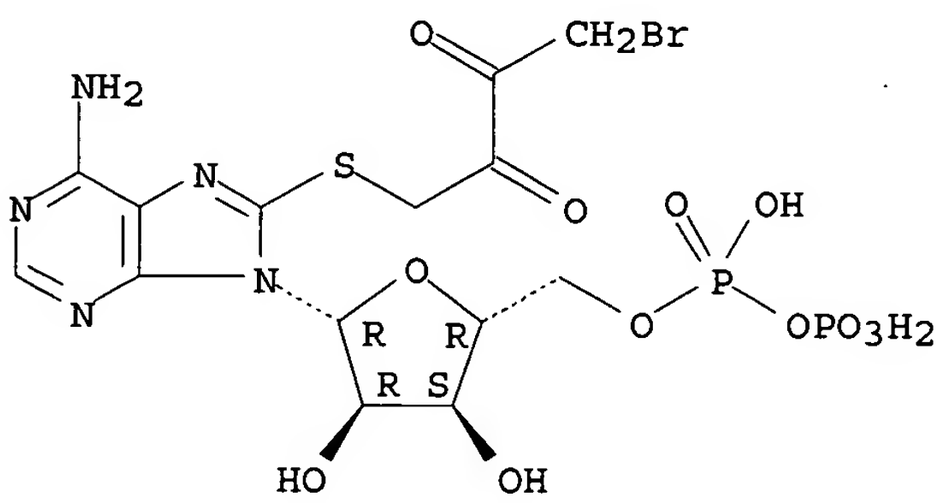
surrounding the identity of an ADP receptor on platelets, we have used an affinity label capable of alkylating a putative exofacial receptor on platelets. We now report that 8-(4-bromo-2,3-dioxobutylthio)adenosine-5'-diphosphate (8-BDB-TADP), which is an analog of the natural ligand ADP, blocked ADP-induced platelet shape change, **aggregation**, exposure of fibrinogen-binding sites, secretion, and calcium mobilization. Following modification by 8-BDB-TADP, the rates of **aggregation** of platelets induced by thrombin, a calcium ionophore (A23187) or a stimulator of protein kinase C (phorbol myristate acetate) were minimally affected. However, the 8-BDB-TADP-modified platelets exhibited decreased rates of **aggregation** in response to ADP, as well as collagen and a thromboxane mimetic (U46619), both of which partially require ADP. Autoradiograms of the gels obtained by SDS-PAGE of solubilized platelets modified by either [β-32P]8-BDB-TADP, or 8-BDB-TADP and NaB[3H]4 showed the presence of a single radiolabeled protein band at 100 kDa. The intensity of this band was reduced when platelets were preincubated with ADP, ATP, and 8-bromo-ADP prior to labeling by the radioactive 8-BDB-TADP. The results show that 8-BDB-TADP selectively and covalently labeled aggregin (100 kDa), a putative ADP receptor, resulting in a loss of ADP-induced platelet responses.

IT **115678-78-9**
RL: ARG (Analytical reagent use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(r; ADP-induced platelet responses inhibition by covalent modification of aggregin by (bromodioxobutylthio)ADP)

RN 115678-78-9 CAPLUS

CN Adenosine 5'-(trihydrogen diphosphate), 8-[(4-bromo-2,3-dioxobutyl)thio]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1994:695525 CAPLUS

DN 121:295525

TI Characterization of the HeLa Cell DNA Polymerase α-Associated Ap4A Binding Protein by Photoaffinity Labeling

AU Baxi, Mayur D.; McLennan, Alexander G.; Vishwanatha, Jamboor K.

CS Medical Center, University of Nebraska, Omaha, NE, 68198-4525, USA

SO Biochemistry (1994), 33(48), 14601-7
CODEN: BICHAW; ISSN: 0006-2960

PB American Chemical Society

DT Journal

LA English

AB The ubiquitous dinucleotide, diadenosine tetraphosphate (Ap4A), has been proposed to be involved in DNA replication and cell proliferation, DNA repair, platelet **aggregation**, and vascular tonus. A protein binding to Ap4A is associated with a multiprotein form of DNA polymerase-α (I) in HeLa cells. Here, the I-associated Ap4A-binding protein (II) was purified to homogeneity. II was resolved into 2 polypeptides of 45 and 22 kDa, designated A1 and A2, resp. [α-32P]8-azido (N3)-Ap4A was used to label purified II, and by crosslinking the photoaffinity label it was determined that Ap4A binds to the A1 subunit. No binding to the ligand was observed with the A2 subunit. Photoaffinity labeling was saturated with .apprx.0.4 μM photolabel, with a

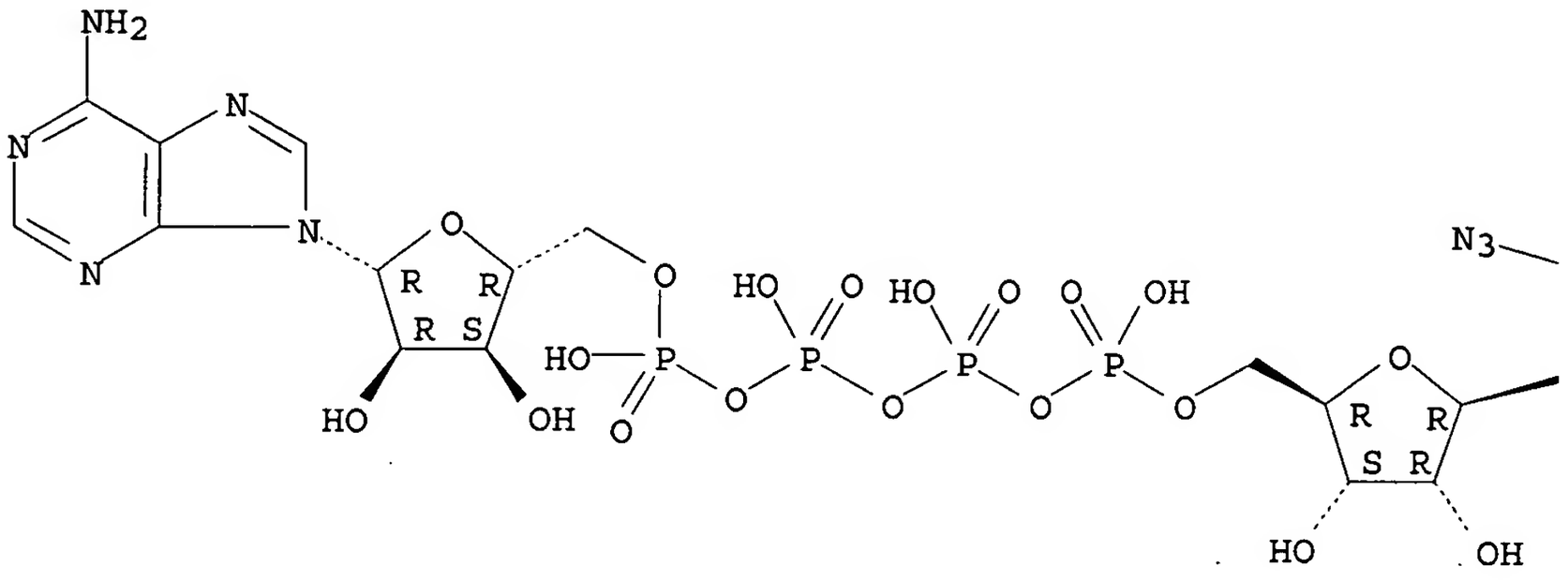
half-maximal binding at 0.15 μM. The labeling was UV-dependent and was competed by both 8-N3-Ap4A and Ap4A. Photoaffinity labeling was not affected by the presence of dATP and dGTP, and was reduced only in the presence of excess of ATP, indicating the specificity of II for Ap4A. Of the diadenosine polyphosphates, Ap4A and Ap5A competed for binding, whereas Ap2A and Ap3A did not compete for binding. Further, the presence of ≥1 adenosine(s) may be necessary since Ap4G competed but Gp4G did not compete for binding to II. Various methylene bisphosphonate and thiophosphate analogs of Ap4A were tested for their effect on photoaffinity labeling with 8-N3-Ap4A. Significant differences were observed among the various analogs in their ability to prevent the photoaffinity labeling of the ligand to II.

IT **126813-90-9**, 8-Azido-Ap4A
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(purification and photoaffinity labeling of HeLa cell DNA polymerase-α-associated Ap4A-binding protein)

RN 126813-90-9 CAPLUS

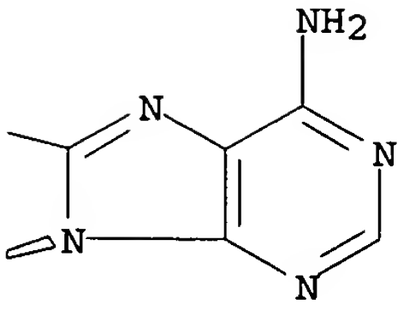
CN Adenosine 5'-(pentahydrogen tetraphosphate), 8-azido-, P'''→5'-ester with adenosine (9CI) (CA INDEX NAME)

Absolute stereochemistry.



PAGE 1-A

PAGE 1-B



L7 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1994:401198 CAPLUS
DN 121:1198
TI Interaction of Nucleotides with Acidic Fibroblast Growth Factor (FGF-1)
AU Chavan, Ashok J.; Haley, Boyd E.; Volkin, David B.; Marfia, Kimberly E.; Verticelli, Adeline M.; Bruner, Mark W.; Draper, Jerome P.; Burke, Carl J.; Middaugh, C. Russell
CS College of Pharmacy, University of Kentucky, Lexington, KY, 40536, USA
SO Biochemistry (1994), 33(23), 7193-202
CODEN: BICHAW; ISSN: 0006-2960
DT Journal

LA English

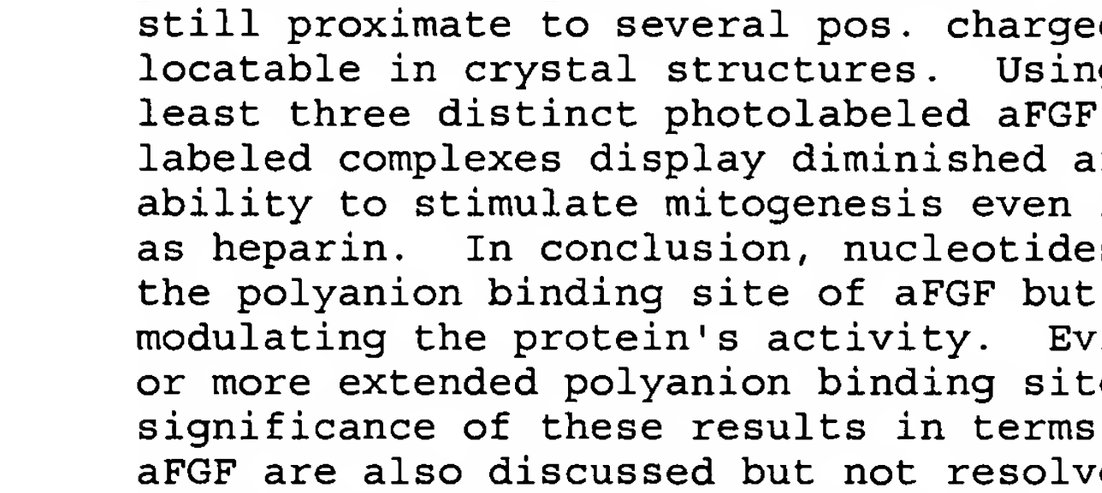
AB A wide variety of nucleotides is shown to bind to acidic fibroblast growth factor (aFGF) as demonstrated by their ability to inhibit the heat-induced **aggregation** of the protein; to enhance the thermal stability of aFGF as monitored by both intrinsic fluorescence and CD; to interact with fluorescent nucleotides and displace a bound polysulfated naphthylurea compound, suramin; to reduce the size of heparin-aFGF complexes; and to protect a reactive aFGF thiol group. The binding of mononucleotides, diadenosine compds. (ApnA), and inorg. polyphosphates to aFGF is enhanced as the degree of phosphorylation of these anions is increased with the presence of the base reducing the apparent binding affinity. The nature of the base appears to have much less effect. Photoactivatable nucleotides (8N3-ATP, 2N3-ATP, 8N3-GTP, and 8N3-Ap4A) were employed to covalently label the aFGF nucleotide binding site. In general, Kd's in the low micromolar range are observed Protection against 90% displacement is observed at several hundred micromolar nucleotide concentration Using 8N3-ATP as a prototypic reagent, photolabeled aFGF was proteolyzed with trypsin and chymotrypsin, and labeled peptides were isolated and sequenced resulting in the identification of 10 possible labeled amino acids (Y8, G20, H21, T61, K112, K113, S116, R119, R122, H124). On the basis of the crystal structure of bovine aFGF, eight of the prospective labeled sites appear to be dispersed around the perimeter of the growth factor's presumptive polyanion binding site. One residue (T61) is more distally located but still proximate to several pos. charged residues, and another (Y8) is not locatable in crystal structures. Using heparin affinity chromatog., at least three distinct photolabeled aFGF species were resolved. These labeled complexes display diminished affinity for heparin and a reduced ability to stimulate mitogenesis even in the presence of polyanions such as heparin. In conclusion, nucleotides bind apparently nonspecifically to the polyanion binding site of aFGF but nevertheless are capable of modulating the protein's activity. Evidence for the presence of a second or more extended polyanion binding site and the potential biol. significance of these results in terms of potential natural ligands of aFGF are also discussed but not resolved.

IT **53696-59-6**, 8-Azido-ATP **65114-35-4**, 8-Azido-GTP
126813-90-9, 8-Azido-Ap4A
RL: BIOL (Biological study)
(acidic fibroblast growth factor binding of, sites for)

RN 53696-59-6 CAPLUS

CN Adenosine 5'-(tetrahydrogen triphosphate), 8-azido- (9CI) (CA INDEX NAME)

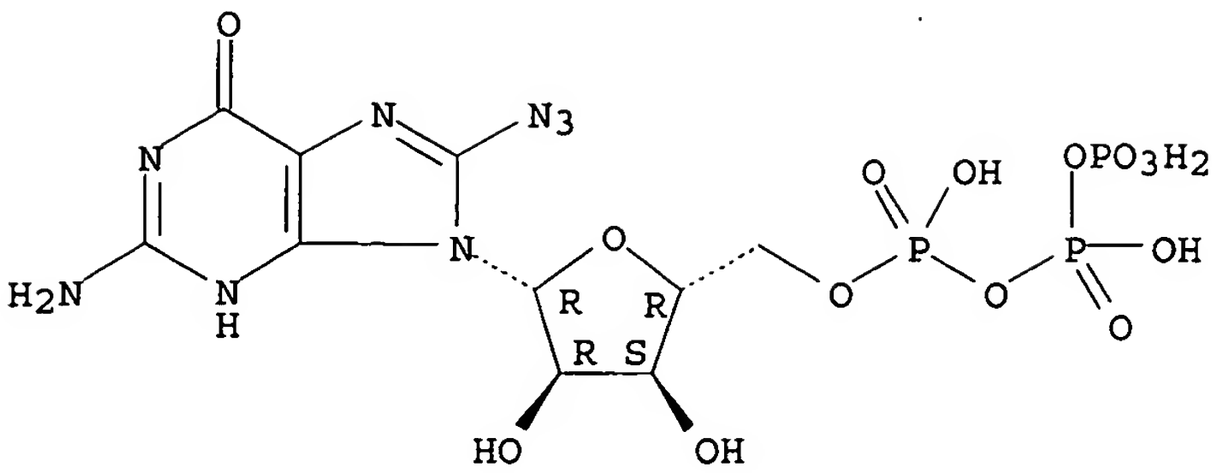
Absolute stereochemistry.



RN 65114-35-4 CAPLUS

CN Guanosine 5'-(tetrahydrogen triphosphate), 8-azido- (9CI) (CA INDEX NAME)

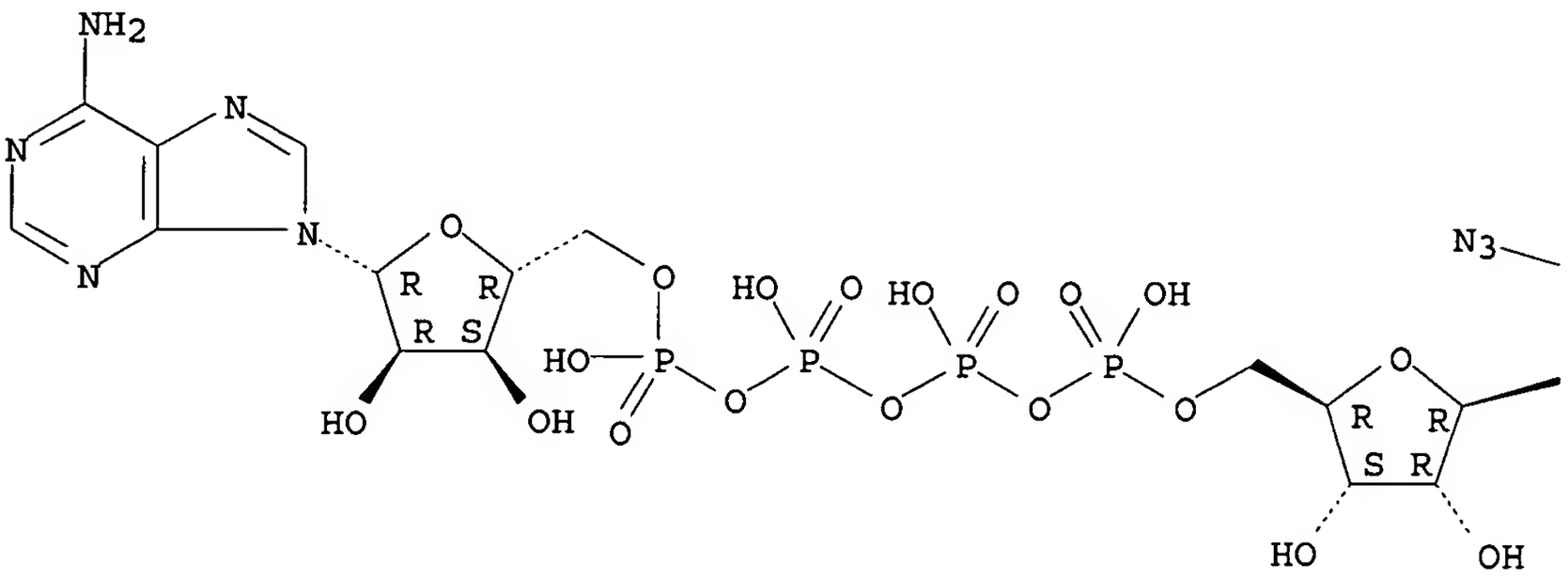
Absolute stereochemistry.



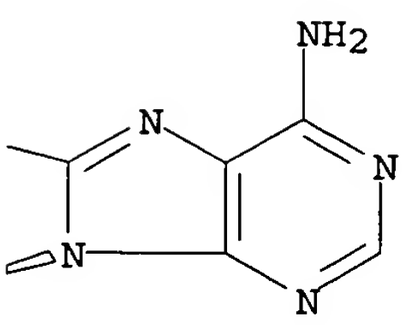
RN 126813-90-9 CAPLUS
CN Adenosine 5'-(pentahydrogen tetraphosphate), 8-azido-, P'''→5'-ester with adenosine (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



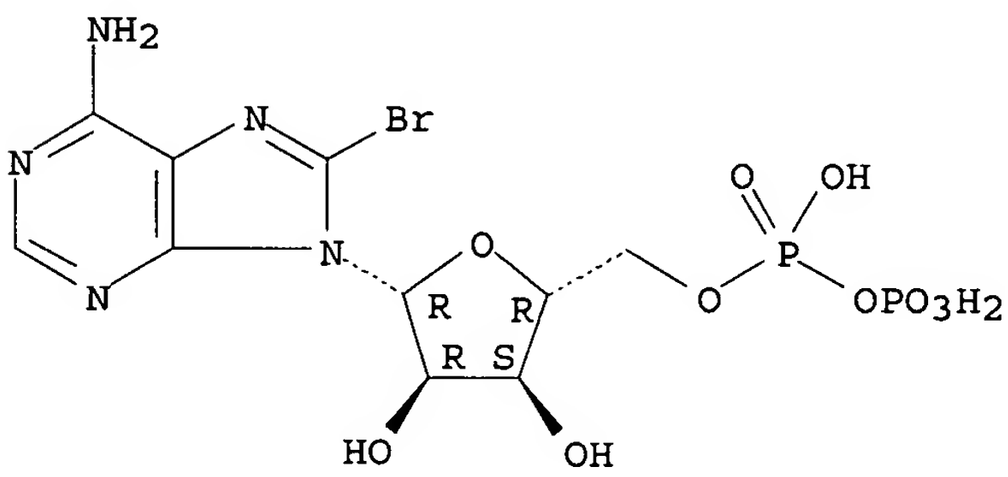
L7 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1993:490701 CAPLUS
DN 119:90701
TI Identification of a receptor for ADP on blood platelets by photoaffinity labeling
AU Cristalli, Gloria; Mills, David C. B.
CS Sch. Med., Temple Univ., Philadelphia, PA, 19140, USA
SO Biochemical Journal (1993), 291(3), 875-81
CODEN: BIJOAK; ISSN: 0306-3275
DT Journal
LA English
AB The synthesis of a new analog of ADP, 2-(p-azidophenyl)-ethylthioadenosine 5'-diphosphate (AzPET-ADP), is described. This compound contains a photolabile phenylazide group attached to the ADP mol. by a thioether link at the purine 2 position. It has been prepared in radioactive form with 32P

in the β-phosphate at a specific radioactivity of 100 mCi/μmol. The reagent activated platelets, causing shape change and **aggregation**, with somewhat lower affinity than ADP. On photolysis the affinity was increased. The reagent also inhibited platelet adenylate cyclase stimulation by prostaglandin E1, with considerably higher affinity than ADP. On photolysis the affinity was decreased. AzPET-ADP competitively inhibited the binding of 2-methylthio[β-32P]ADP, a ligand for the receptor by which ADP causes inhibition of adenylate cyclase. In the dark, AzPET-[β-32P]ADP bound reversibly and with high affinity to a single population of sites similar in number to the sites that bind 2-methylthiol[β-32P]ADP. Binding was inhibited by ADP and by ATP and by p-chloromercuribenzenesulfonic acid (pCMBS). On exposure to UV light in the presence of platelets, AzPET-[β-32P]ADP was incorporated covalently but non-specifically into several platelet proteins, although prominent intracellular proteins were not labeled. Specific labeling was confined to a single region of SDS/polyacrylamide gels, overlying but not comigrating with actin. Incorporation of radioactivity into this region was inhibited by ADP and by ATP as well as by ADPβS, ATPαS and pCMBS, but not by adenosine, GDP or AMP. Inhibition of AzPET-[β-32P]ADP incorporation was closely correlated with inhibition of equilibrium binding of 2-methylthio[β-32P]ADP. These results suggest that the labeled protein, which migrates with an apparent mol. mass of 43 kDa in reduced gels, is the receptor through which ADP inhibits adenylate cyclase.

IT **23600-16-0**
RL: ANST (Analytical study)
(binding of azidophenylethylthioadenosine diphosphate and methylthio ADP into protein in blood platelets in relation to)

RN 23600-16-0 CAPLUS
CN Adenosine 5'-(trihydrogen diphosphate), 8-bromo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



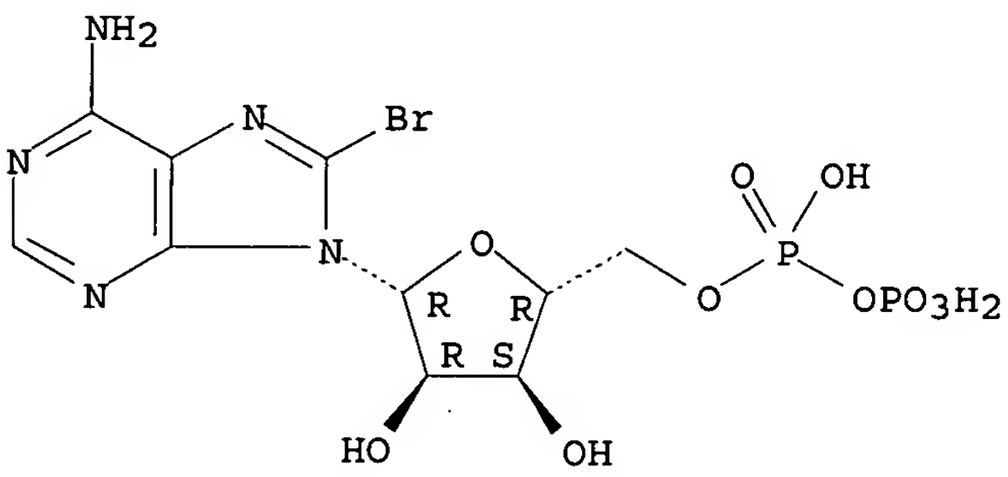
L7 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1991:464361 CAPLUS
DN 115:64361
TI The effect of agonists and antagonists of platelet **aggregation** on von Willebrand factor-mediated platelet agglutination
AU McPherson, Jean; Zucker, Marjorie B.; Mauss, Evelyn A.; Brownlea, Sandra
CS Fac. Med., Univ. Newcastle, Newcastle, 2308, Australia
SO Thrombosis and Haemostasis (1991), 65(5), 573-7
CODEN: THHADQ; ISSN: 0340-6245
DT Journal
LA English
AB Ristocetin-induced platelet agglutination (RIPA) in EDTA-treated citrated platelet-rich plasma was reduced to 49% by 1.25 μM ADP, 41% by 1 μM A23187, and 26% by 0.1 μg/mL platelet activating factor (PAF). The effect of 5-110 μM epinephrine was not dose-dependent, but varied between donors, with RIPA from 56-100% of the control. The inhibitory effects of these agonists were not altered by prior treatment of platelets with aspirin. Prior addition of 200 μM ATP (an ADP receptor antagonist acting at both high- and low-affinity ADP receptors) prevented the inhibitory action of ADP but not that of A23187 or PAF, suggesting that the inhibitory actions of the latter were not mediated by released ADP. As 700 μM 8-bromoadenosine 5-diphosphate (an ADP receptor antagonist

acting mainly at the high-affinity receptor) did not prevent the ADP-induced inhibition of RIPA, the interaction of ADP with the low-affinity receptor was presumably responsible for its inhibitory action. As A23187, but not phorbol myristate acetate (0.1 μM), inhibited RIPA, an increase in intracellular calcium ions rather than direct stimulation of protein kinase C appears to mediate the agonist-induced inhibition. Cytochalasin B (10.5-21 μM), dibucaine (0.5-1 mM), and PGE1 (25 nM) added before or after the agonist prevented or reversed the ADP-, A23187-, and PAF-induced inhibition of RIPA, suggesting that the state of the platelet cytoskeleton affects the inhibition. N-Ethylmaleimide (0.25-0.5 mM), an agent that can penetrate cell membranes and block sulfydryl groups, prevented or reversed the ADP-, A23187- and PAF-induced inhibition of RIPA, but 0.5 mM dithionitrobisbenzoic acid, a non-penetrating sulfydryl blocker, had no effect. Diamide (0.1-0.5 mM), an agent that can crosslink cytoskeletal proteins by oxidation of sulfydryl groups, reduced RIPA. Thus, an increase in intracellular calcium ions with resultant cytoskeletal changes and reorganization of intracellular sulfydryl groups may mediate the inhibitory action of agonists on RIPA.

IT **23600-16-0**, 8-Bromo-ADP
RL: BIOL (Biological study)
(blood platelet **aggregation** induced by ristocetin response to)

RN 23600-16-0 CAPLUS
CN Adenosine 5'-(trihydrogen diphosphate), 8-bromo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



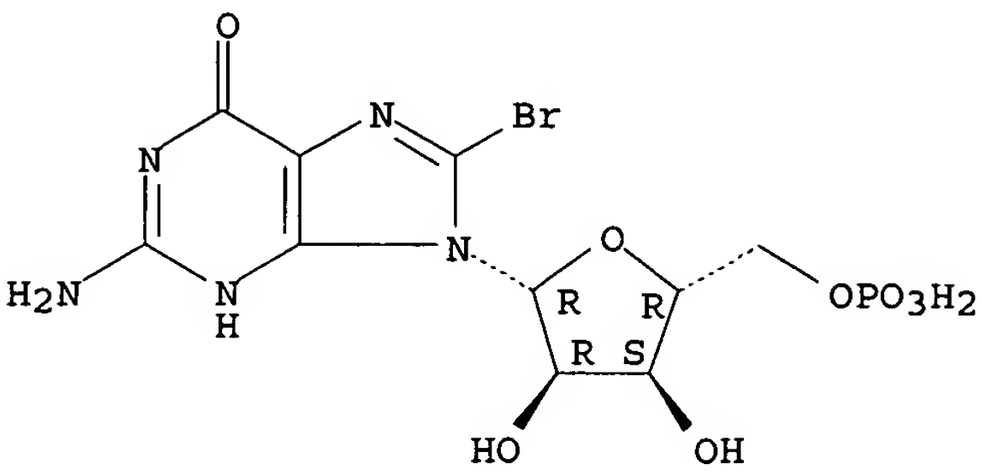
L7 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1989:511319 CAPLUS
DN 111:111319
TI The role of nucleotide self-**aggregation** on the interaction process between clupeine YI (a fish protamine) and mono- and dinucleotides
AU Andini, Salvatore; Ferrara, Luciano; Cocozziello, Beatrice; De Napoli, Lorenzo; Piccialli, Gennaro; Barbato, Stefania
CS Dip. Chim., Univ. Napoli, Naples, I-80134, Italy
SO Gazzetta Chimica Italiana (1989), 119(5), 271-5
CODEN: GCITA9; ISSN: 0016-5603
DT Journal
LA English
AB The interaction between clupeine YI and various nucleotides in aqueous solution has been investigated with the aim of understanding the reason for the stronger affinity of purinic nucleotides towards the protein as compared with pyrimidinic ones. The study has been performed by 1H NMR spectrometry by adding increasing amts. of nucleotide to the protamine solution The results obtained suggest that it is not the nature (purinic or pyrimidinic) of the nucleotide but its ability to give rise to a self-**aggregation** process that is crucial in the interaction with the protein. In fact, nucleotide complexation should provide a polyanionic matrix around which the protein can be strongly linked. This model was tested with different natural, synthetic, and modified nucleotides and with some dinucleotides.

IT **21870-09-7**, 8-Bromo-5'-gmp **23567-96-6**, 8-Bromo-5'-amp **61286-93-9**
RL: BIOL (Biological study)

(protamine clupeine Y1 interaction with, nucleotide self-**aggregation** role in)

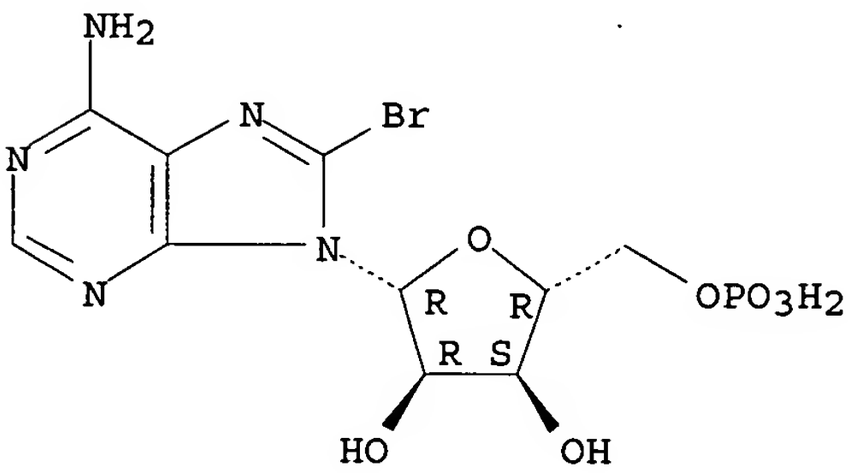
RN 21870-09-7 CAPLUS
CN 5'-Guanylic acid, 8-bromo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



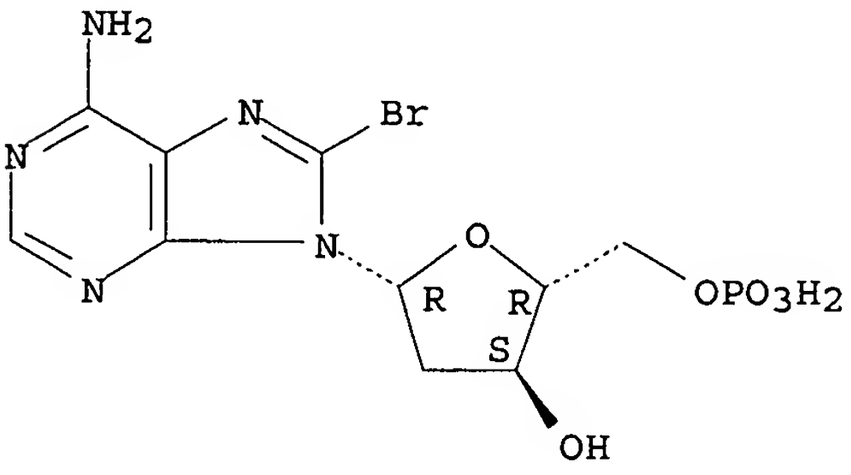
RN 23567-96-6 CAPLUS
CN 5'-Adenylic acid, 8-bromo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



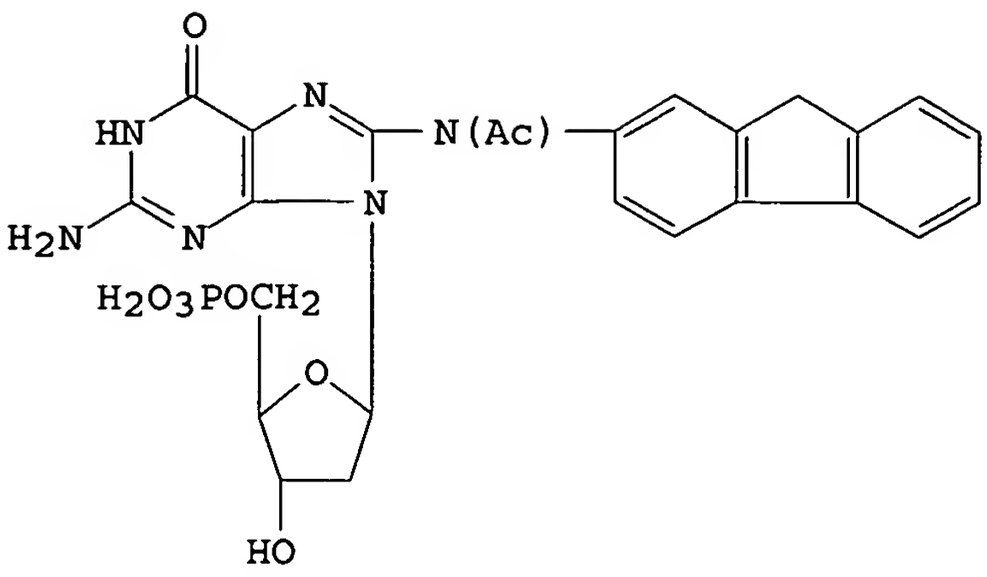
RN 61286-93-9 CAPLUS
CN 5'-Adenylic acid, 8-bromo-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1986:437246 CAPLUS
DN 105:37246
TI Proton NMR study of self-association and restricted internal rotation of the C8-substituted deoxyguanosine 5'-monophosphate adduct of the carcinogen 2-(acetylamino)fluorene
AU Evans, Frederick E.; Miller, Dwight W.; Levine, Robert A.
CS Div. Chem., Natl. Cent. Toxicol. Res., Jefferson, AR, 72079, USA
SO Journal of Biomolecular Structure & Dynamics (1986), 3(5), 935-48
CODEN: JBSDD6; ISSN: 0739-1102
DT Journal
LA English

GI



I

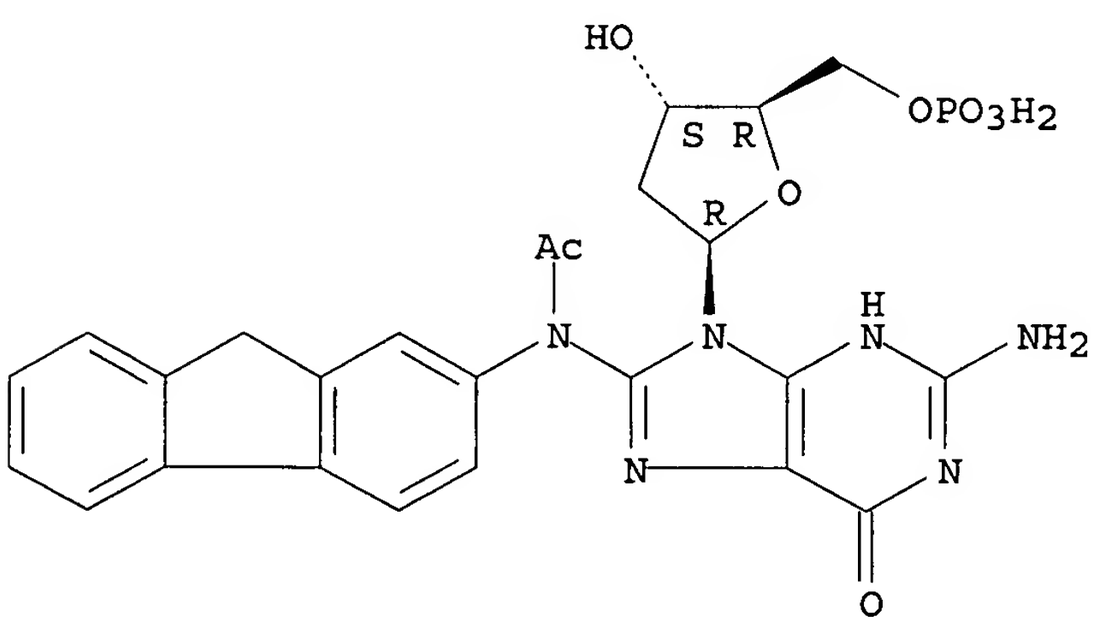
AB The high-field 1H NMR spectra of a nucleotide-carcinogen adduct formed from 2-(acetylamino)fluorene, [8-(N-fluoren-2-ylacetamido)-2'-deoxyguanosine 5'-monophosphate (I) [**14490-86-9**]], was examined in aqueous solution as a function of concentration at high and low temps. An anomalous concentration dependence of NMR spectra was observed at >1 mM. These spectral characteristics were analyzed in terms of changes in selfassocn. and in the interconversions between torsional diastereomers associated with the central N. Association consts. were computed. Stacking interactions, which involve the fluorene and guanine rings, are strong, cooperative and highly temperature-dependent. Deacetylation alters the mode of stacking. Several effects of solvent and **aggregation** on the conformation at the central N are discussed.

IT **14490-86-9**
RL: BIOL (Biological study)
(NMR study of structure of)

RN 14490-86-9 CAPLUS

CN 5'-Guanylic acid, 8-(acetyl-9H-fluoren-2-ylamino)-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1986:84344 CAPLUS

DN 104:84344

TI Distances between active site probes in glutamine synthetase from Escherichia coli: fluorescence energy transfer in free and in stacked dodecamers

AU Maurizi, Michael R.; Kasprzyk, Philip G.; Ginsburg, Ann

CS Lab. Mol. Biol., Natl. Cancer Inst., Bethesda, MD, 20205, USA

SO Biochemistry (1986), 25(1), 141-51
CODEN: BICHAW; ISSN: 0006-2960

DT Journal

LA English

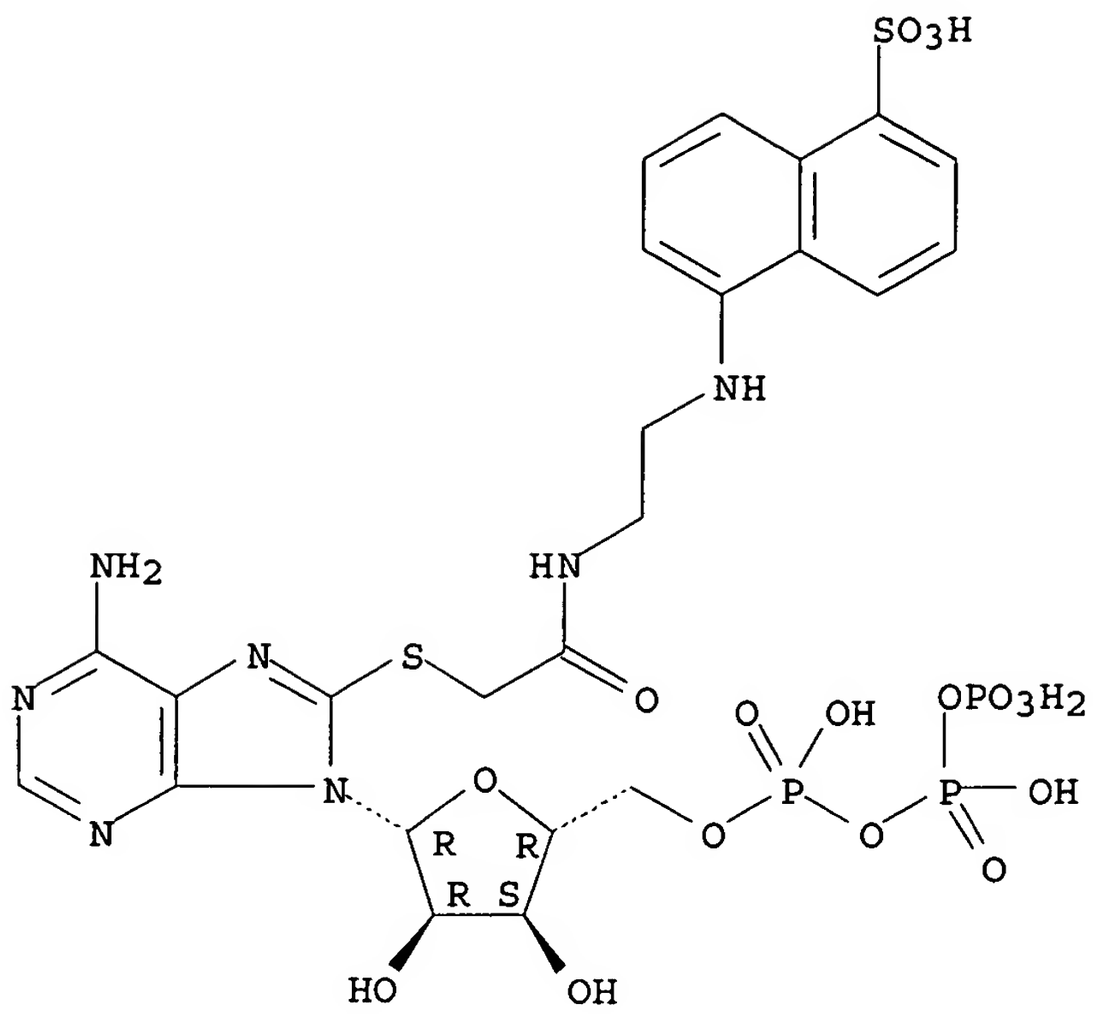
AB Probes for fluorescence energy transfer measurement were introduced into active sites of dodecameric glutamine synthetase from Escherichia coli by substituting appropriate ATP analogs for ATP in the autoinactivation reaction of this enzyme with L-methionine-(S)-sulfoximide and Mn2+. Two fluorescent donors, 8-mercapto-ATP alkylated with either 5-[[[(iodoacetyl)amino]ethyl]amino]naphthalene-1-sulfonic acid (AEDANS-ATP) or 1,N6-etheno-2-aza-ATP (aza-ε-ATP), and 2 acceptors, 6-mercaptopurine ribonucleotide triphosphate or 8-mercapto-ATP alkylated with the chromophore [[(4-dimethylamino)phenyl]azo]-2-iodoanilide (6-Y- or 8-Y-ATP), were used. Fluorescence emissions of enzyme derivs. with 1 or 2 equivalent of fluorescent donor/dodecamer and either an acceptor (Y) or ADP at the remaining active sites were compared at pH 7.0. The results, together with the known geometry of the enzyme, indicate that active-site probes in the dodecamer are widely separated and that energy transfer occurs from a single donor to 2 or 3 acceptors on adjacent subunits. The calculated distance between equidistant active-site probes on heterologously bonded subunit within the same hexagonal ring is 56-60 Å. Probes on isologously boned subunits are no closer than 60 Å and may be as far apart as 78 Å. Thus, active sites are away from the 6-fold axis of symmetry toward the outer edges of the dodecamer and are located ≥30 Å from the plane separating the hexagonal rings. During Zn2+-induced stacking of the same enzyme derivs. along the 6-fold axes of symmetry, addnl. quenches of fluorescence probes were dependent on the presence of acceptors on sep. dodecamers. The Zn2+-induced face-to-face **aggregation** of dodecamers in the presence of 46 μM ZnCl2 and 9 mM MgCl2 at pH 7.0 and an Arrhenius activation energy of 22.3 kcal/mol and a 2nd-order rate constant at 25° of .apprx.105 M-1 s-1 at early stages. Time-dependent fluorescence quenches maximum values of 47-70% quench when the average oligomer was dodecamers. After correction for unquenched polymer ends, a fluorescent donor and an acceptor probe in layered dodecamers were estimated to be .apprx.36 Å apart (an average value if there is some twisting of single strands). This intermol. energy-transfer distance confirms that activity-site nucleotide probes are located toward exterior surfaces away from the lateral plane separating hexagonal rings of a dodecamer.

IT **99376-89-3**
RL: BIOL (Biological study)
(fluorescence energy transfer to acceptor from, in glutamine synthetase of Escherichia coli)

RN 99376-89-3 CAPLUS

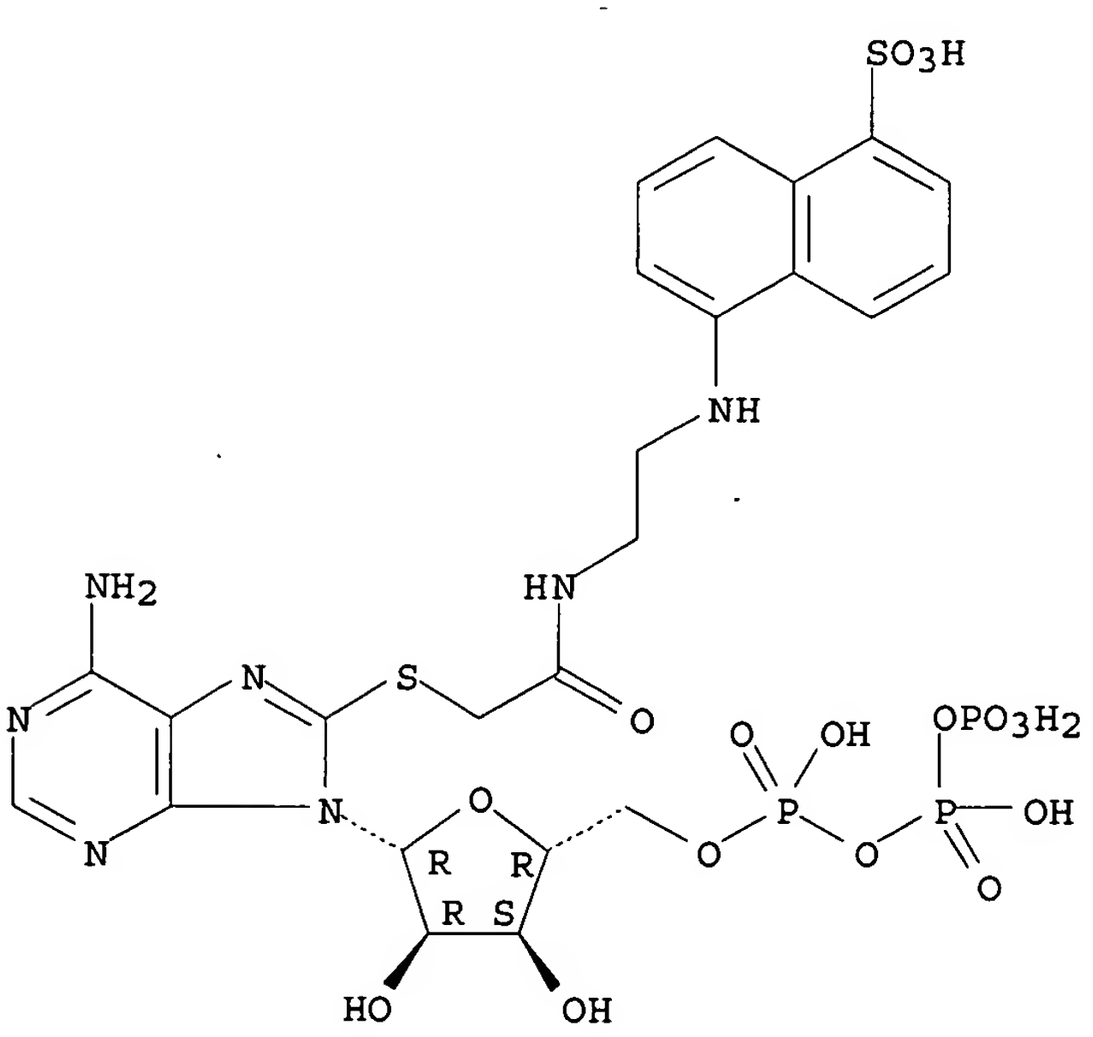
CN 1-Naphthalenesulfonic acid, 5-[[2-[[[[6-amino-9-[5-O-[hydroxy[[hydroxy(phosphonooxy)phosphinyl]oxy]phosphinyl]-β-D-ribofuranosyl]-9H-purin-8-yl]thio]acetyl]amino]ethyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **99376-89-3D**, reaction products with glutamine synthetase
RL: PRP (Properties)
(fluorescence of)
RN 99376-89-3 CAPLUS
CN 1-Naphthalenesulfonic acid, 5-[[2-[[[[6-amino-9-[5-O-[hydroxy[[hydroxy(phosphonooxy)phosphinyl]oxy]phosphinyl]-β-D-ribofuranosyl]-9H-purin-8-yl]thio]acetyl]amino]ethyl]amino]- (9CI) (CA INDEX NAME)

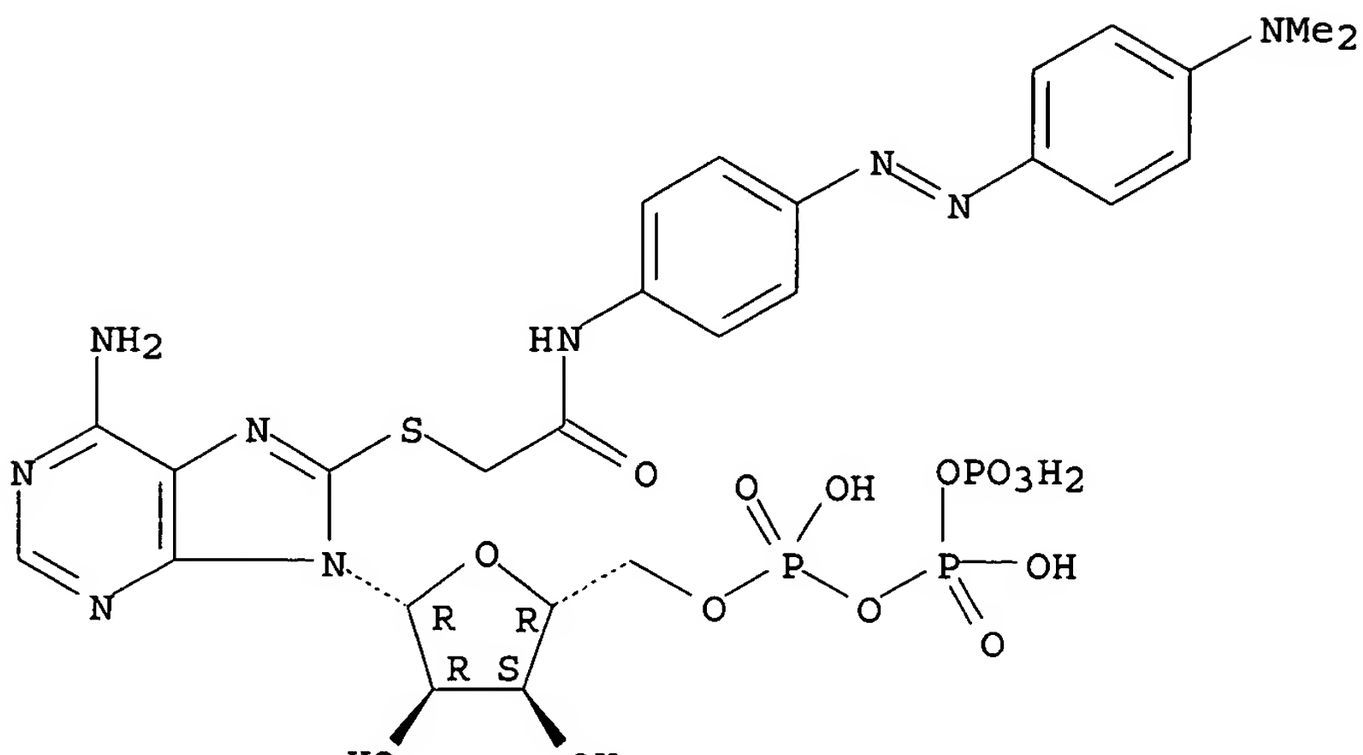
Absolute stereochemistry.



IT **99376-91-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and use in glutamine synthetase active site of Escherichia coli anal.)
RN 99376-91-7 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-[[2-[[4-[[4-

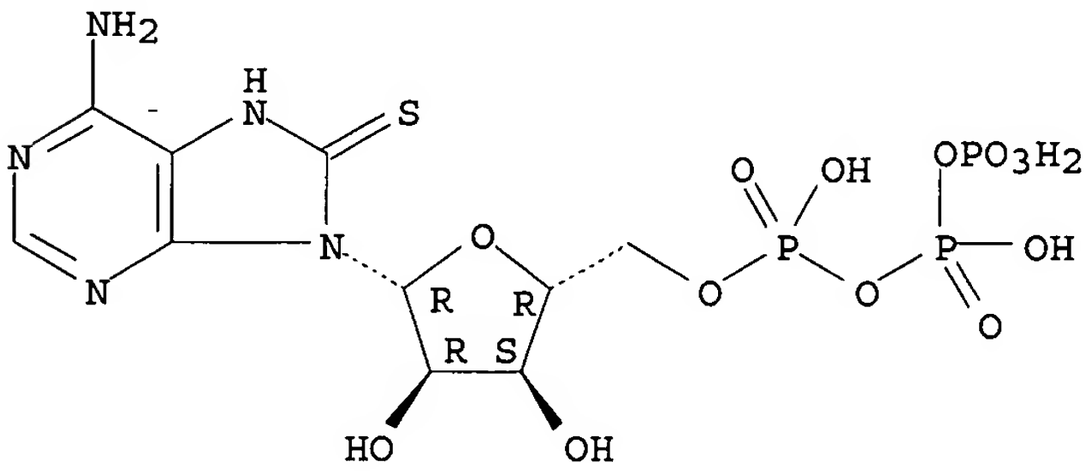
(dimethylamino)phenyl]azo]phenyl]amino]-2-oxoethyl]thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



IT **41106-66-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with iodoacetanilide derivative)
RN 41106-66-5 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 7,8-dihydro-8-thioxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

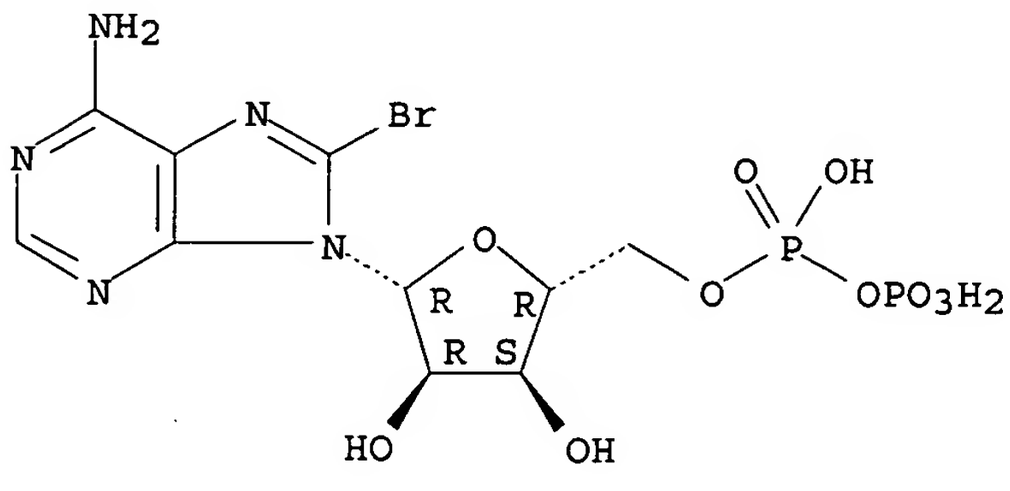


L7 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1983:519886 CAPLUS
DN 99:119886
TI Interactions of two ADP analogs, xanthosine-5'-diphosphate and 8-bromoadenosine-5'-diphosphate, and ADP with citrated human platelet-rich plasma
AU Ragatz, Barth H.
CS Sch. Med., Indiana Univ., Fort Wayne, IN, 46805, USA
SO Proceedings of the Indiana Academy of Science (1982), Volume Date 1981, 91, 183-7
CODEN: PIACAP; ISSN: 0073-6767
DT Journal
LA English
AB To determine the stereochem. nature of the ADP receptor of human platelets, the interaction of 2 ADP analogs (xanthosine 5'-diphosphate (XDP) and 8-bromo-ADP) with human platelet-rich plasma was investigated. XDP over a 100-fold concentration range failed to yield any competitive inhibition of ADP-induced platelet **aggregation**. Completely analogous results were observed for bromo-ADP. When either compound was preincubated with the platelet-rich plasma for 5 min prior to ADP addition, no inhibition of

ADP-induced **aggregation** occurred. Thus, substituents at position C-2 and C-6 (as seen with XDP) and C-8 (bromo-ADP) are not tolerated at the ADP receptor.

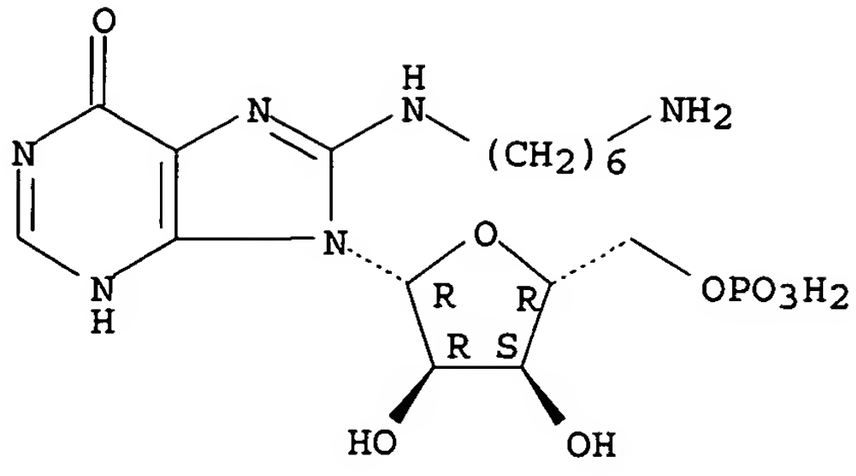
IT **23600-16-0**
RL: BIOL (Biological study)
(ADP receptors stereochem. in human blood platelet in relation to)
RN 23600-16-0 CAPLUS
CN Adenosine 5'-(trihydrogen diphosphate), 8-bromo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



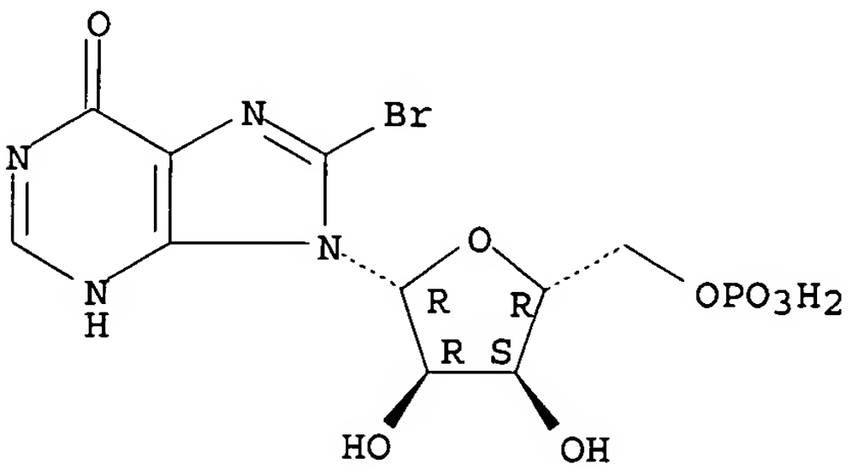
L7 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1980:582136 CAPLUS
DN 93:182136
TI Affinity chromatography on immobilized nucleotides. The synthesis, specificity and applications of immobilized inosine 5'-monophosphate
AU Clonis, Yannis D.; Lowe, Christopher R.
CS Dep. Biochem., Univ. Southampton, Southampton, UK
SO European Journal of Biochemistry (1980), 110(1), 279-88
CODEN: EJBCAI; ISSN: 0014-2956
DT Journal
LA English
AB The synthesis and characterization of 2 IMP analogs, 8-(6-aminohexyl)-IMP and inosine 2',3'-O-[1-(6-aminohexyl)-levulinic acid amide]-acetal 5'-monophosphate are described. These analogs were attached to CNBr-activated agarose through the terminal NH2 group of the spacer mol. The immobilized IMP analogs displayed specificity for the inosine-nucleotide-dependent enzyme IMP dehydrogenase but not for the NAD+-dependent enzymes L-alanine and L-acetate dehydrogenases. Escherichia coli IMP dehydrogenase could be eluted biospecifically from immobilized 8-substituted and ribose-substituted IMP adsorbents with IMP, XMP, and GMP. Multiple peaks of enzyme activity in the elution profiles were interpreted in terms of **aggregation** of the enzyme. A protocol for the large-scale purification of E. coli IMP dehydrogenase is proposed. Homogeneous enzyme of sp. activity 9.1 units/mg was obtained in 50% overall yield, representing 14 mg pure protein from a 20-L culture of E. coli. The 2 IMP analogs were inactive as substrates in the IMP dehydrogenase reaction.
IT **75204-34-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and immobilization of, on Sepharose for affinity chromatog.)
RN 75204-34-1 CAPLUS
CN 5'-Inosinic acid, 8-[(6-aminohexyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



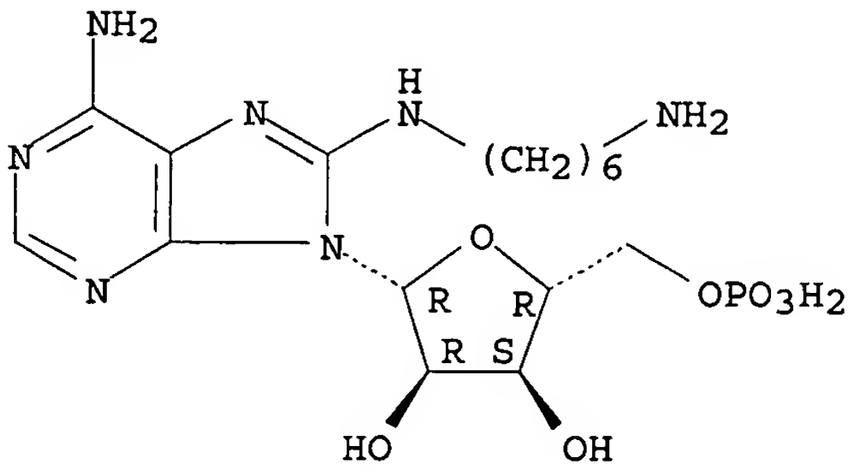
IT **75204-33-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with diaminohexane)
RN 75204-33-0 CAPLUS
CN 5'-Inosinic acid, 8-bromo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

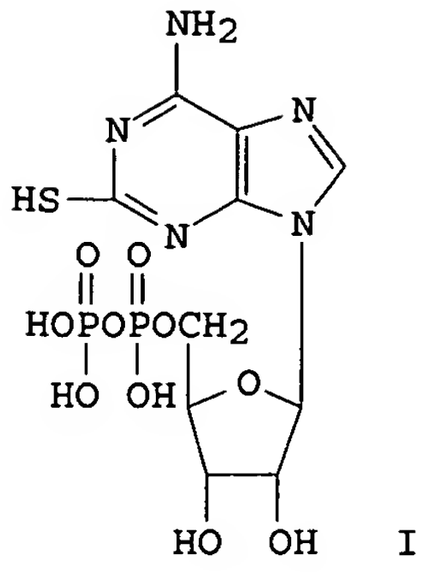


IT **52977-32-9DP**, reaction products with Sepharose 4B
RL: PREP (Preparation)
(preparation of, for affinity chromatog.)
RN 52977-32-9 CAPLUS
CN 5'-Adenylic acid, 8-[(6-aminohexyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1976:472930 CAPLUS
DN 85:72930
TI Sulfhydryl analogs of adenosine diphosphate: chemical synthesis and activity as platelet-aggregating agents
AU Stone, J. V.; Singh, Raj K.; Horak, H.; Barton, P. G.
CS Dep. Biochem., Univ. Alberta, Edmonton, AB, Can.
SO Canadian Journal of Biochemistry (1976), 54(6), 529-33
CODEN: CJBIAE; ISSN: 0008-4018
DT Journal
LA English
GI



I

AB 2-Thioadenosine 5'-diphosphate (2-SH ADP)(I) [59924-53-7], 2,2'-dithiobisadenosine 5'-diphosphate (2,2'-(S-ADP)2) [59924-54-8], 8-thioadenosine 5'-diphosphate triethylammonium salt (8SH ADP) [**59924-56-0**], and 6-mercaptopurineriboside 5'-disphosphate (6-MPRDP) [805-63-0] were synthesized as potential affinity labels for ADP receptors on the blood-platelet membrane. The mean relative activities of these compds. in aggregating human platelets suspended in homologous plasma were 155% (2,2'-(S-ADP)2), 74% (2-SH ADP), 0.65% (8-SH ADP), and 0.08% (6-MPRDP). The mean relative activities against washed platelets were 249% (2,2'-(S-ADP)2) and 115% (2-SHADP), whereas no **aggregation** occurred with 8-SH ADP or 6-MPRDP. The last 2 compds. were weak inhibitors of ADP-induced **aggregation**. Therefore, thio-substitution at postion 2 followed by oxidation to a disulfide appears to be the most promising approach to further studies of affinity labeling of membrane ADP-receptors.

IT **59924-56-0P**
RL: PREP (Preparation)
(preparation and blood platelet **aggregation** response to)

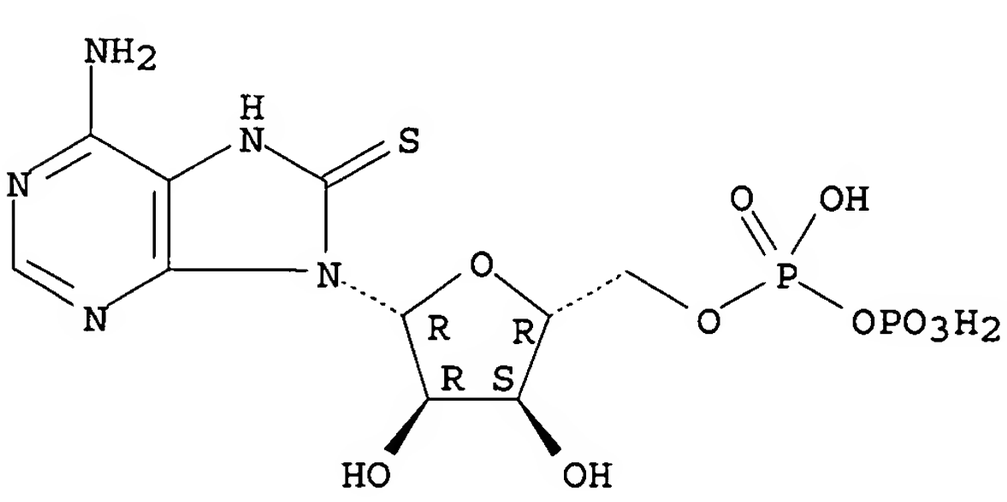
RN 59924-56-0 CAPLUS

CN Adenosine 5'-(trihydrogen diphosphate), 7,8-dihydro-8-thioxo-, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

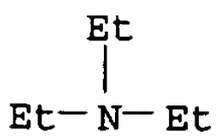
CRN 59924-55-9
CMF C10 H15 N5 O10 P2 S

Absolute stereochemistry.



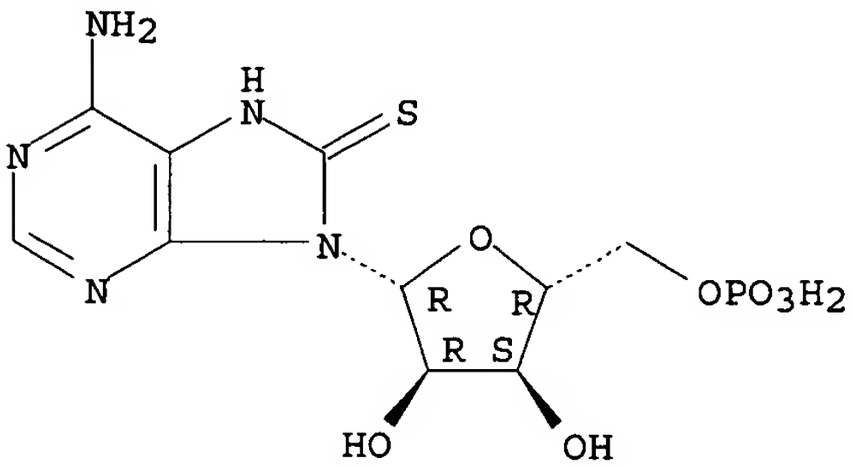
CM 2

CRN 121-44-8
CMF C6 H15 N



IT **34051-09-7P**
RL: PREP (Preparation)
(preparation of)
RN 34051-09-7 CAPLUS
CN 5'-Adenylic acid, 7,8-dihydro-8-thioxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	79.69	246.84

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-10.50	-10.50

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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 19, 2006 (20060519/UP).

10/620,520

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     FILE 'REGISTRY' ENTERED AT 08:47:22 ON 13 MAY 2006
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L2             20 S L1 SSS SAM
L3                STRUCTURE UPLOADED
L4             19 S L3 SSS SAM

     FILE 'REGISTRY' ENTERED AT 09:08:57 ON 13 MAY 2006
L5                STRUCTURE UPLOADED
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L7             32 S L5 SSS FULL

     FILE 'CAPLUS' ENTERED AT 09:10:18 ON 13 MAY 2006
L8             17 S L7

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           128 NTPDASE
                 (NTPDASE OR NTPDASES)
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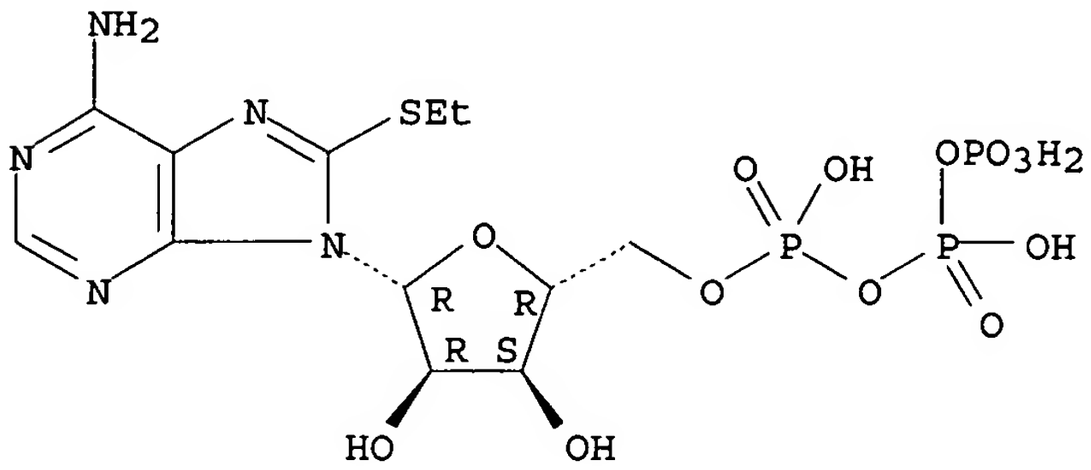
L9   ANSWER 1 OF 5  CAPLUS  COPYRIGHT 2006 ACS on STN
AN   2004:911398  CAPLUS
DN   142:214281
TI   C8-substituted purine nucleotide analogs and their use as inhibitors of
     nucleoside triphosphate diphosphohydrolases
IN   Halbfinger, Efrat; Fischer, Bilha; Beaudoin, Adrien R.; Gendron, Fernand
     Pierre
PA   Universite de Sherbrooke, Can.; Bar-Ilan University
SO   Can. Pat. Appl., 54 pp.
     CODEN: CPXXEB
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.          DATE
     ---------------     ----   --------    --------------------     --------
PI   CA 2311084           AA    20011209    CA 2000-2311084          20000609
PRAI CA 2000-2311084             20000609
OS   CASREACT 142:214281
AB   Ectonucleoside triphosphate diphosphohydrolases [NTPDases; EC
     3.6.1.5] constitute a family of enzymes which are involved in the metabolism
     of extracellular nucleotides, catalyzing the hydrolysis of the gamma and
     beta phosphate bonds of triphospho- and diphosphonucleosides (whereas
     5'-nucleotidases [EC 3.1.3.5] catalyze the hydrolysis of alpha phosphate
     bond of monophosphonucleosides). These extracellular nucleotides interact
     with endothelial, epithelial and smooth muscle cells, as well as blood
     cells and lymphoid cells, to influence the different physiol. systems of
     vertebrates. Since these ecto-nucleotidases alter the extracellular
     concns. of nucleotides these enzymes modulate their physiol. effects,
     including, for example, platelet aggregation, heart function, control of
     vascular tone and inflammation reactions, electrolyte secretion and
     gastrointestinal motility, neurotransmission both in central and
     peripheral nervous systems, as well as other effects in other physiol.
     systems. This invention provides C8 substituted purine nucleotide
     analogs, such as ATP analogs, and further provides their use as inhibitors
     of NTPDases and thereby as tools to modulate the conversion of
     nucleotides into nucleoside derivs., and thus modulate the levels of these
     compds. Such modulation further provides for the modulation of the
     activity and function of many processes which are affected by these
     compds.
IT   81609-35-0P 284040-51-3P 284040-52-4P
     284040-53-5P
     RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);
     SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
     study); PREP (Preparation); USES (Uses)
```

(C8-substituted purine nucleotide analogs and their use as inhibitors of nucleoside triphosphate diphosphohydrolases to modulate purine nucleotide levels and biol. processes)

RN 81609-35-0 CAPLUS

CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(ethylthio)- (9CI) (CA INDEX NAME)

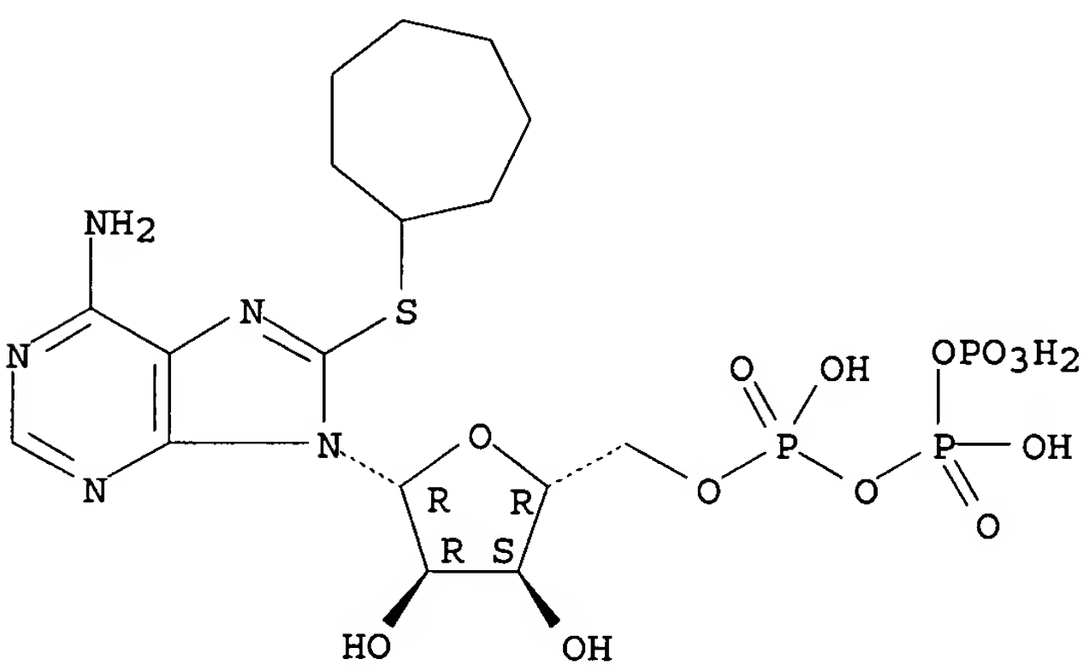
Absolute stereochemistry.



RN 284040-51-3 CAPLUS

CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(cycloheptylthio)- (9CI) (CA INDEX NAME)

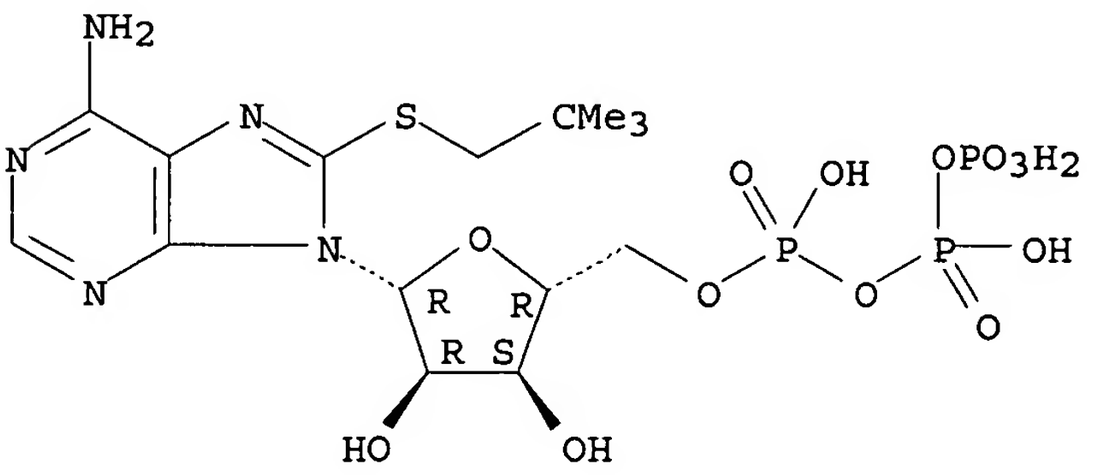
Absolute stereochemistry.



RN 284040-52-4 CAPLUS

CN Adenosine 5'-(tetrahydrogen triphosphate), 8-[(2,2-dimethylpropyl)thio]- (9CI) (CA INDEX NAME)

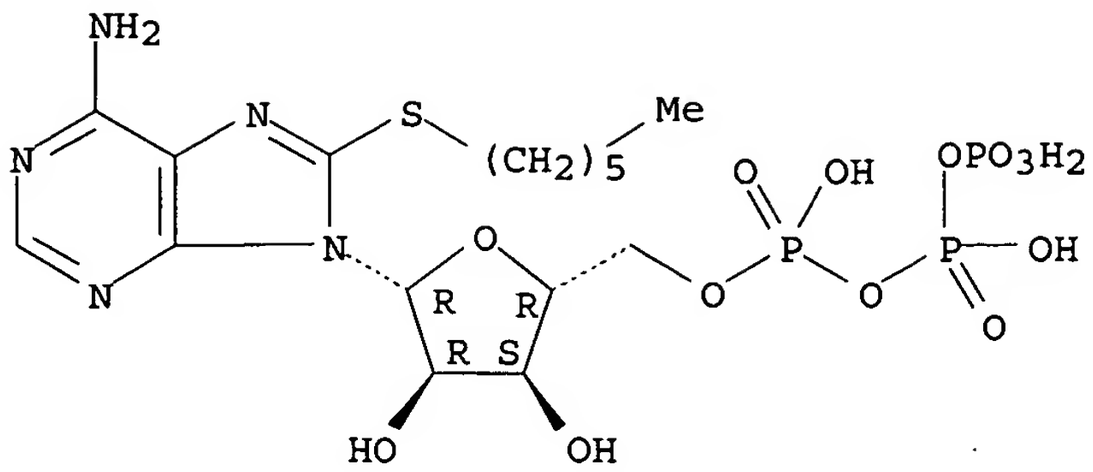
Absolute stereochemistry.



RN 284040-53-5 CAPLUS

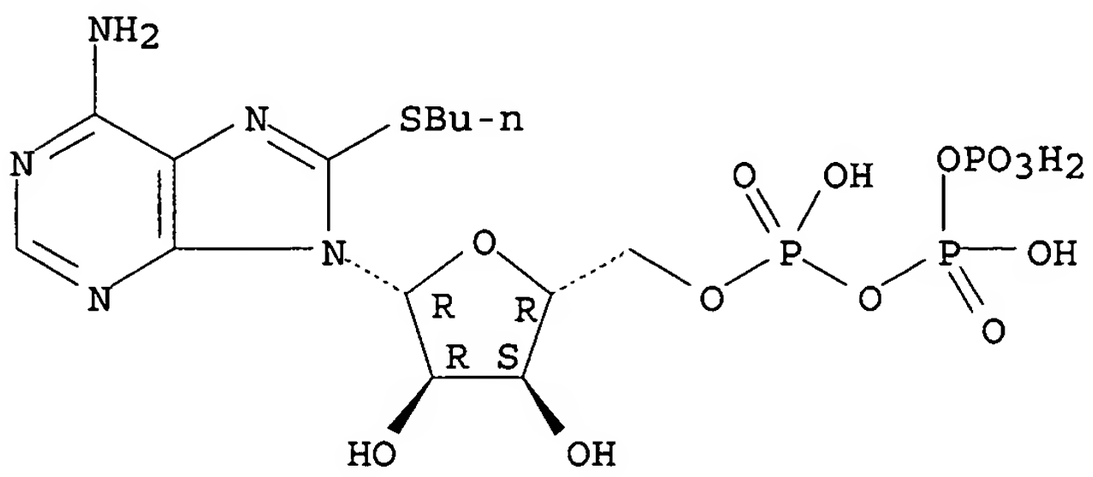
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(hexylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **284040-54-6**
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(C8-substituted purine nucleotide analogs and their use as inhibitors of nucleoside triphosphate diphosphohydrolases to modulate purine nucleotide levels and biol. processes)
RN 284040-54-6 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:856092 CAPLUS
DN 139:333119
TI Ecto-nucleoside triphosphate diphosphohydrolase inhibition-based methods for screening for a compound useful in the treatment or prevention of lymphocytic disorders, for inhibiting lymphocyte activity and preventing or treating lymphocytic disorders
IN Beaudoin, Adrien; Benrezzak, Ouhida
PA Bioflash Inc., Can.
SO PCT Int. Appl., 63 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003089664	A1	20031030	WO 2003-CA583	20030422
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2382768	AA	20031019	CA 2002-2382768	20020419
CA 2479501	AA	20031030	CA 2003-2479501	20030422

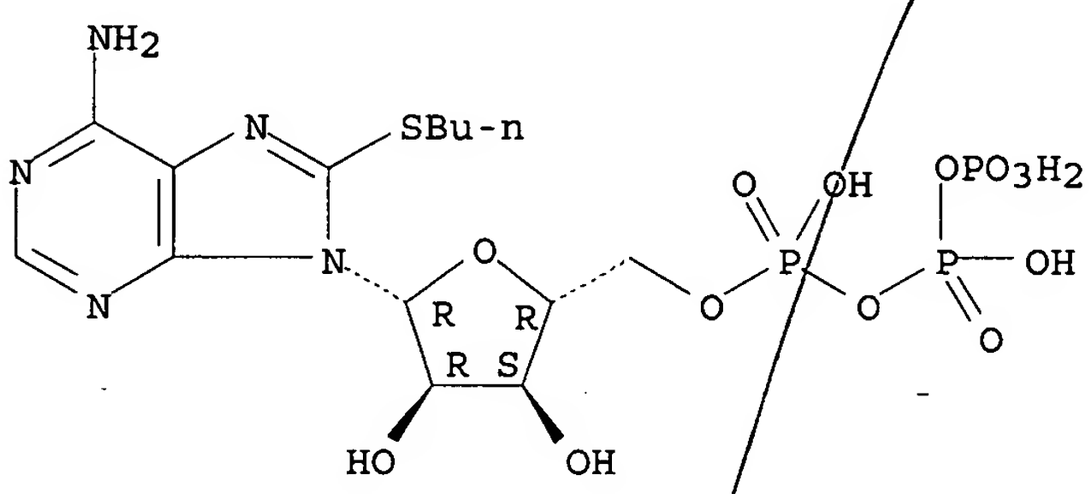
	AU 2003226989	A1	20031103	AU 2003-226989	20030422
	US 2005164306	A1	20050728	US 2003-511133	20030422
PRAI	CA 2002-2382768	A	20020419		
	WO 2003-CA583	W	20030422		

AB The invention discloses a method of screening for a compound useful in the treatment of a disease or condition characterized by an immune cell disorder, wherein the cell expresses ecto-nucleoside triphosphate diphosphohydrolases (**NTPDases**), the method comprising contacting a candidate compound with **NTPDase**, wherein the candidate compound is selected if the activity of the **NTPDase** is reduced in the presence of the candidate compound as compared to that in the absence thereof. The invention also discloses a method for inhibiting an immune cell activity in a mammal, comprising targeting immune cells with an effective amount of a **NTPDase** inhibitor. The invention further discloses a method to prevent or reduce the risk of rejection of transplanted tissue or organ, comprising administering to the animal an effective amount of **NTPDase** inhibitor.

IT **284040-54-6 344402-39-7**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(ecto-nucleoside triphosphate diphosphohydrolase inhibition-based methods for screening for agents for treatment of immune cell disorder-associated conditions)

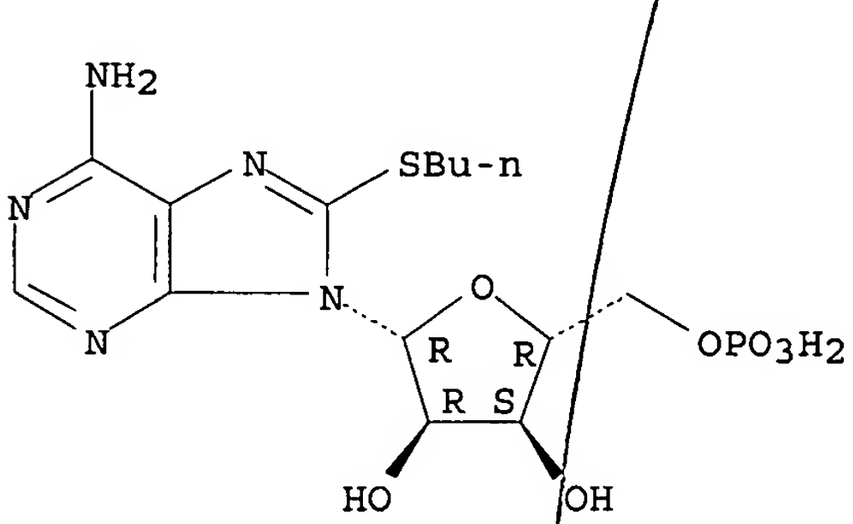
RN 284040-54-6 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 344402-39-7 CAPLUS
CN 5'-Adenylic acid, 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



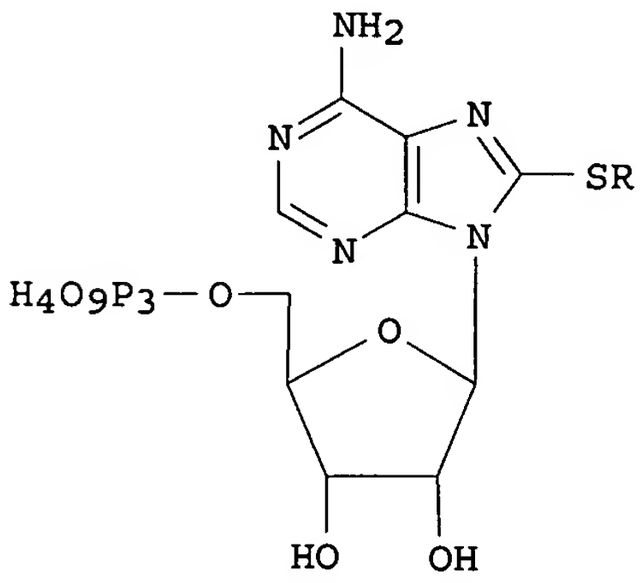
RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:711173 CAPLUS
DN 139:230955
TI Preparation of C8-substituted purine nucleotide analogs as **NTPDase** inhibitors
IN Beaudoin, Adrien R.; Gendron, Fernand-Pierre; Halbfinger, Efrat; Fischer,

Bilha
PA Bar-Ilan University, Israel; Universite De Sherbrooke
SO U.S., 21 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6617439	B1	20030909	US 2000-591177	20000609
	US 2004043955	A1	20040304	US 2003-620520	20030716
PRAI	US 2000-591177	A3	20000609		

OS MARPAT 139:230955
GI



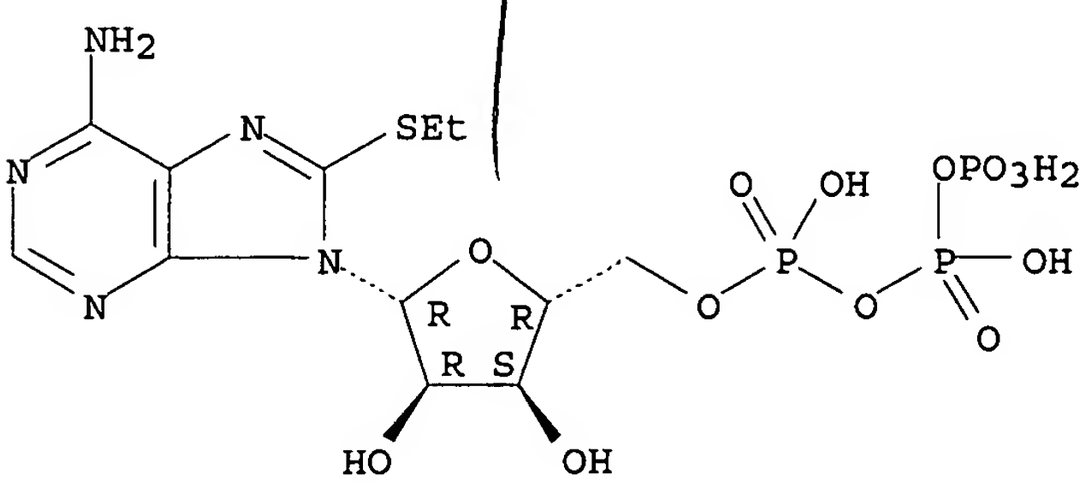
I

AB C8-substituted purine nucleotide analogs, I (R is alkyl, cycloalkyl) such as ATP analogs, and their use is described, including their use as inhibitors of **NTPDases** and thereby as tools to modulate the conversion of nucleotides into nucleoside derivs., and thus modulate the levels of these compds. Such modulation further provides for the modulation of the activity and function of many processes which are affected by these compds. Thus, I [R = (CH2)3Me] was prepared and tested in vivo as NTDPase inhibitor. I [R = (CH2)3Me] interacts specifically with the binding site of the enzyme potentially reduces the risk of interference with other ATP-binding enzymes or receptors, and thus possesses a high degree of specificity. The compds. of the invention were analyzed with resp. to any effects on the activity of purinoceptors.

IT **81609-35-0P 284040-51-3P 284040-52-4P**
284040-53-5P 284040-54-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of C8-substituted purine nucleotide analogs as **NTPDase** inhibitors)

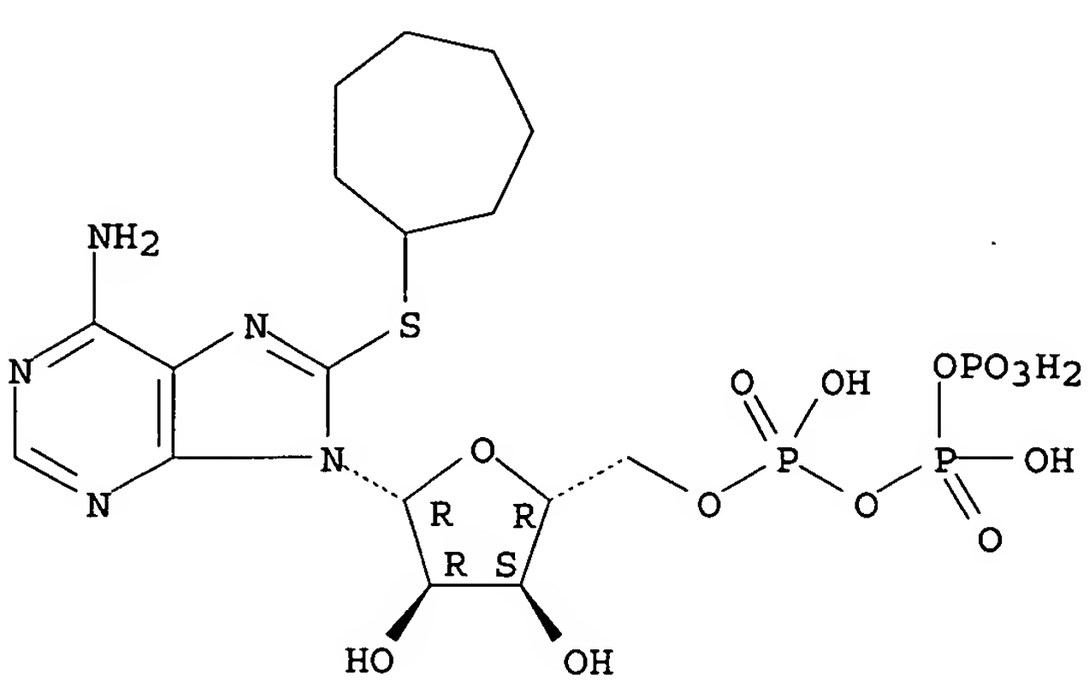
RN 81609-35-0 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(ethylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



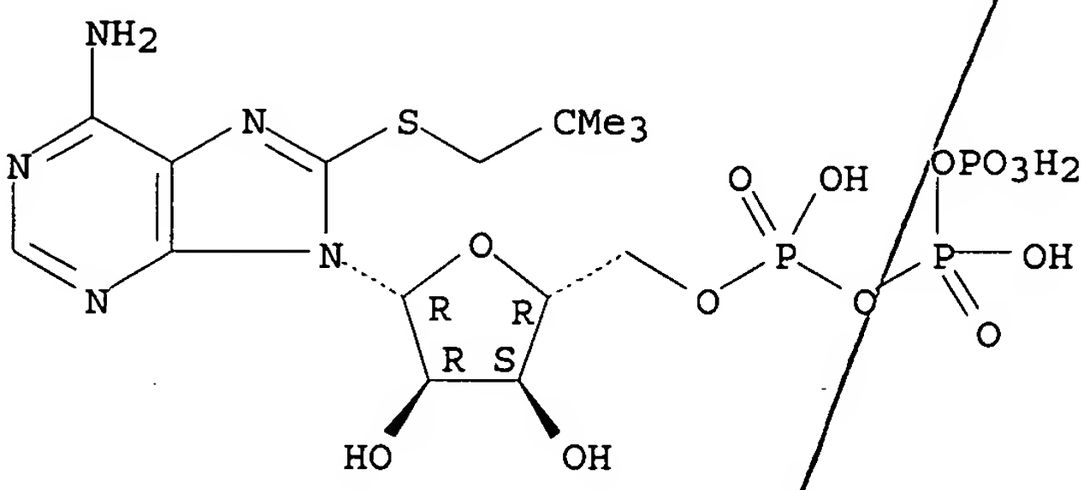
RN 284040-51-3 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(cycloheptylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



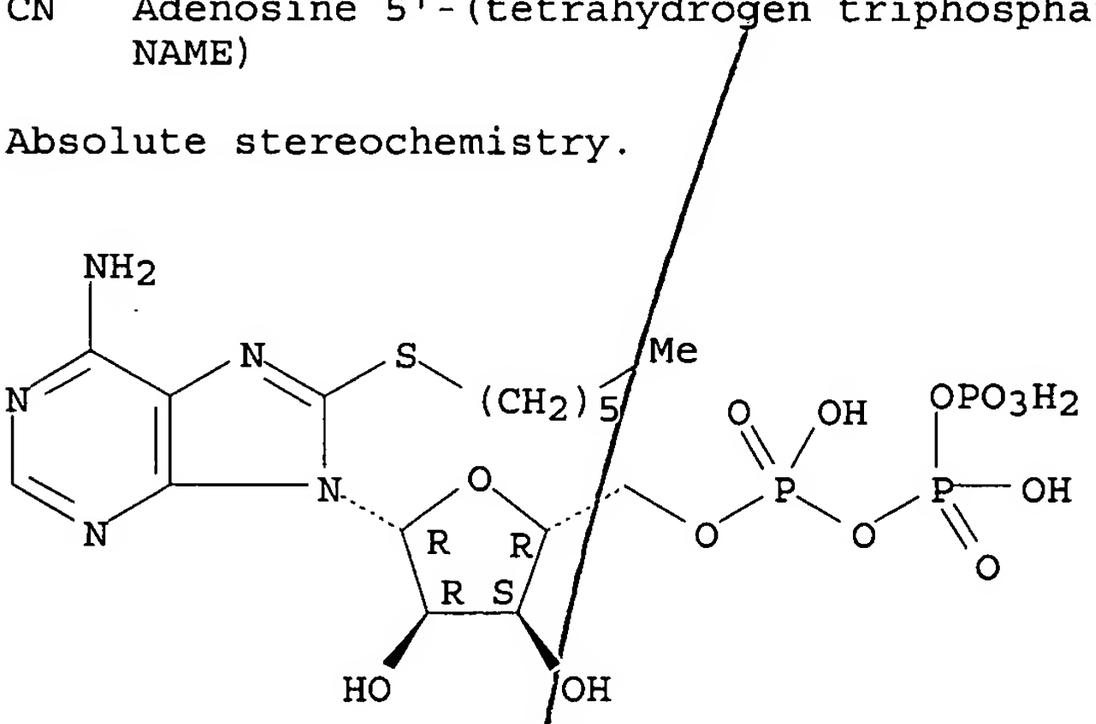
RN 284040-52-4 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-[(2,2-dimethylpropyl)thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



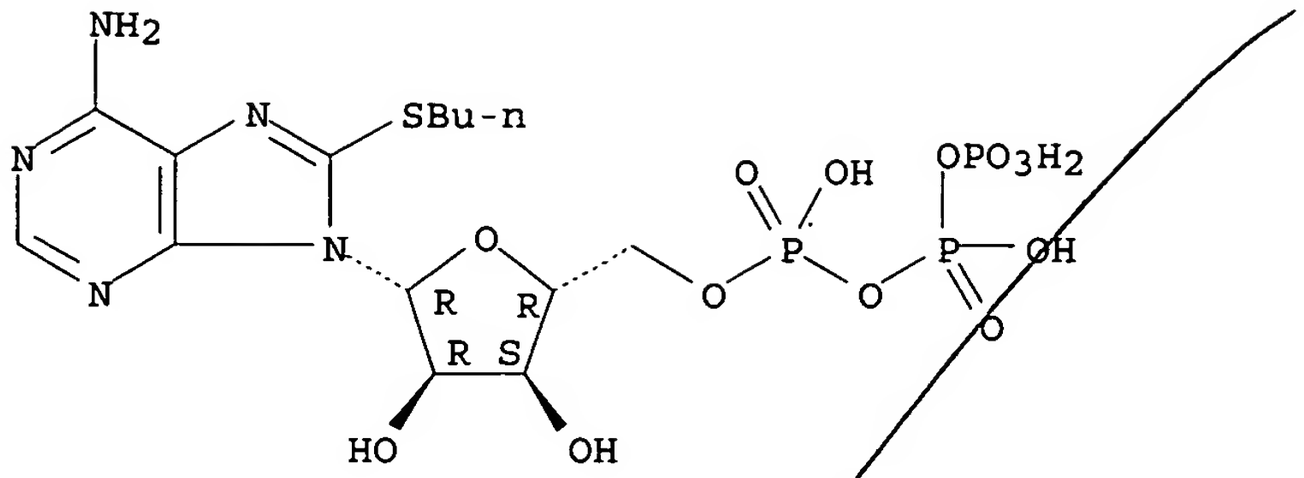
RN 284040-53-5 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(hexylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 284040-54-6 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)- (9CI) (CA INDEX NAME)

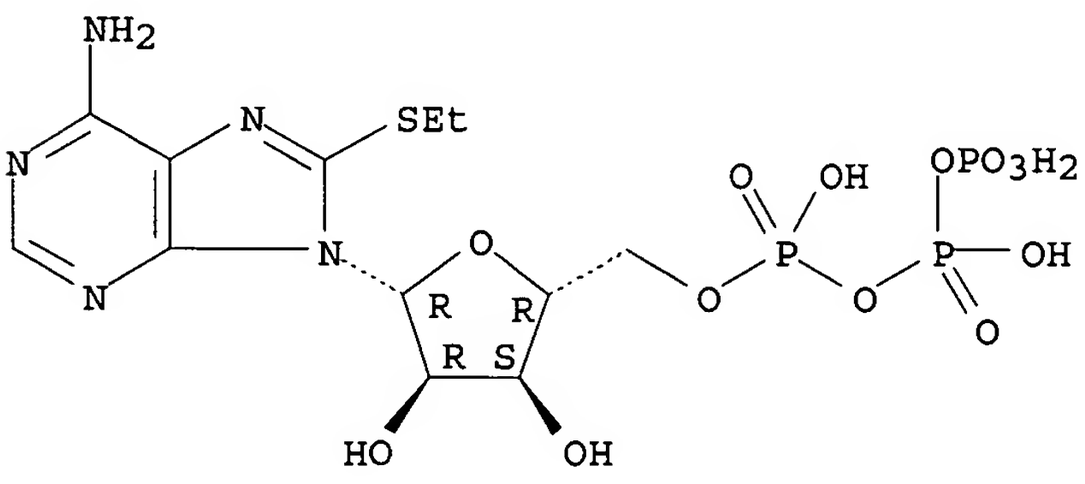
Absolute stereochemistry.



RE.CNT 71 THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

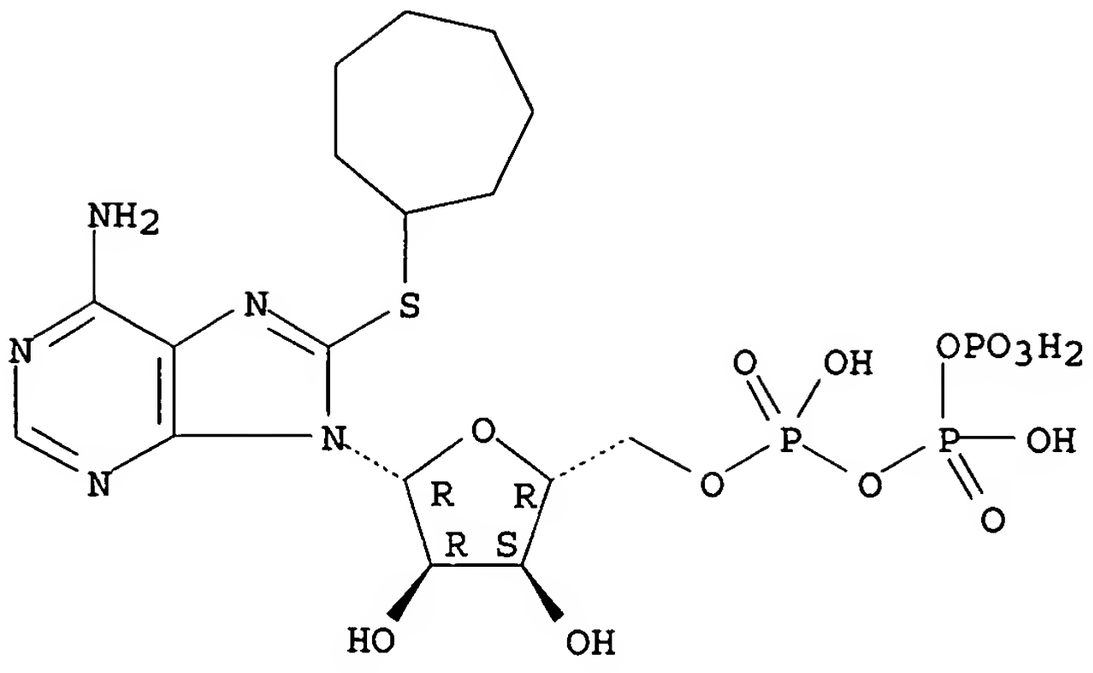
L9 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2001:327844 CAPLUS
DN 135:149038
TI Inhibitors of **NTPDase**: key players in the metabolism of extracellular purines
AU Gendron, F. P.; Halbfinger, E.; Fischer, B.; Beaudoin, A. R.
CS Department of Biology, University of Sherbrooke, Sherbrooke, Can.
SO Advances in Experimental Medicine and Biology (2000), 486(Purine and Pyrimidine Metabolism in Man X), 119-123
CODEN: AEMBAP; ISSN: 0065-2598
PB Kluwer Academic/Plenum Publishers
DT Journal
LA English
AB This study described the potential of a new class of ATP analogs as nucleoside triphosphate diphosphohydrolase (**NTPDase**) inhibitors. From previous studies, 8-thiobutyladenosine 5'-triphosphate (8-BuS-ATP) appears to be a specific and efficient **NTPDase** inhibitor. This novel inhibitor is a new tool to regulate **NTPDase** activity and thereby influencing purine signaling in mammalian.
IT **81609-35-0 284040-51-3 284040-53-5 284040-54-6**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(inhibitors of nucleoside triphosphate diphosphohydrolase - key players in metabolism of extracellular purines)
RN 81609-35-0 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(ethylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



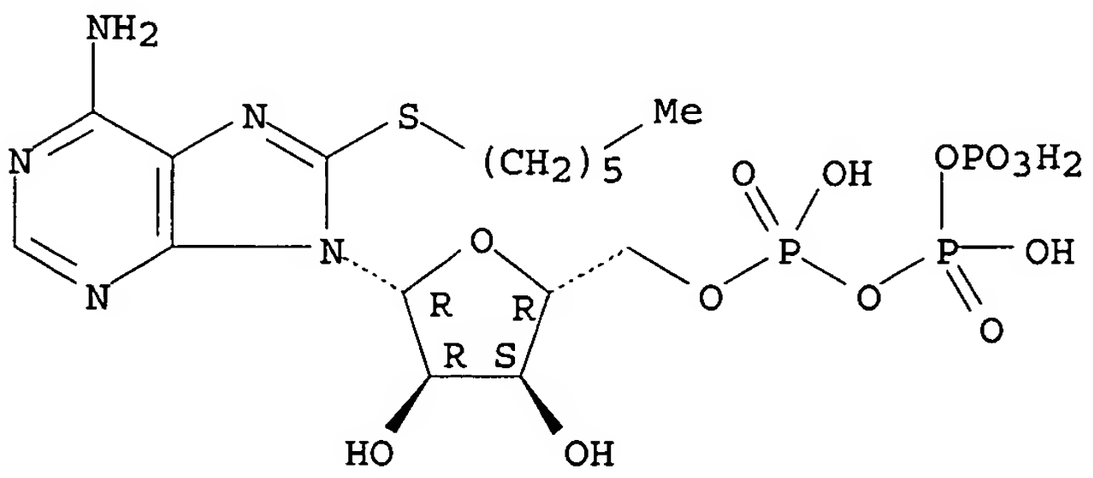
RN 284040-51-3 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(cycloheptylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



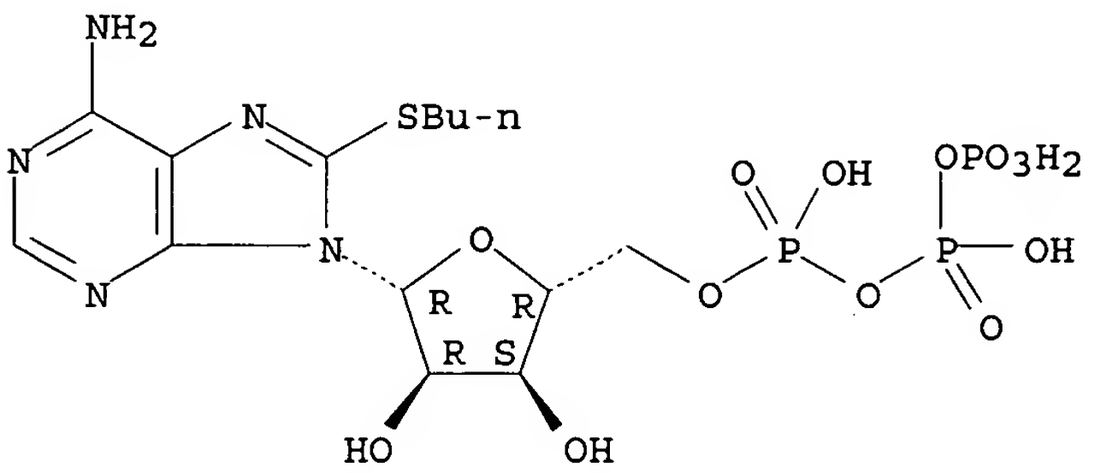
RN 284040-53-5 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(hexylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 284040-54-6 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



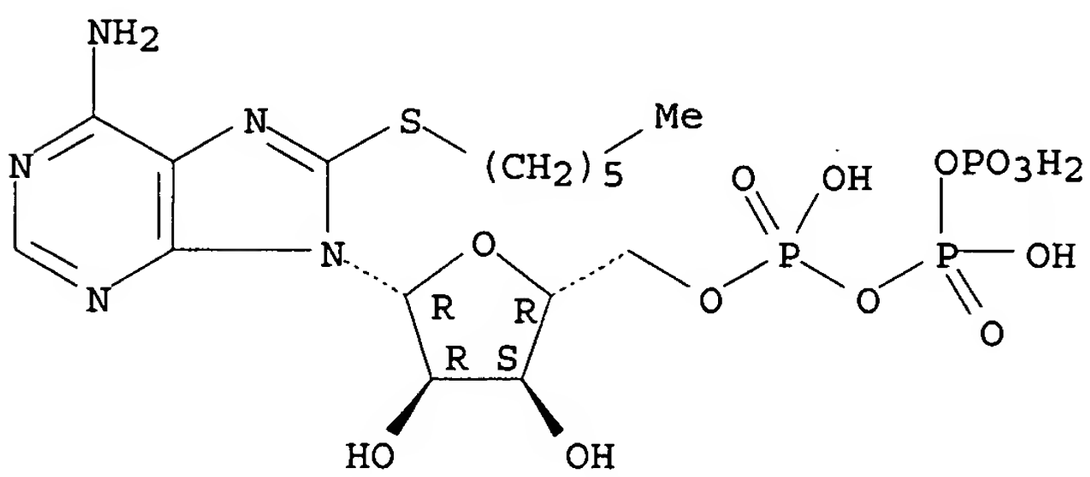
RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2000:304989 CAPLUS
DN 133:105244
TI Novel Inhibitors of Nucleoside Triphosphate Diphosphohydrolases: Chemical Synthesis and Biochemical and Pharmacological Characterizations
AU Gendron, Fernand-Pierre; Halbfinger, Efrat; Fischer, Bilha; Duval, Martine; D'Orleans-Juste, Pedro; Beaudoin, Adrien R.
CS Department de Biologie, Universite de Sherbrooke, Sherbrooke, QC, J1K 2R1, Can.
SO Journal of Medicinal Chemistry (2000), 43(11), 2239-2247
CODEN: JMCMAR; ISSN: 0022-2623

Printed

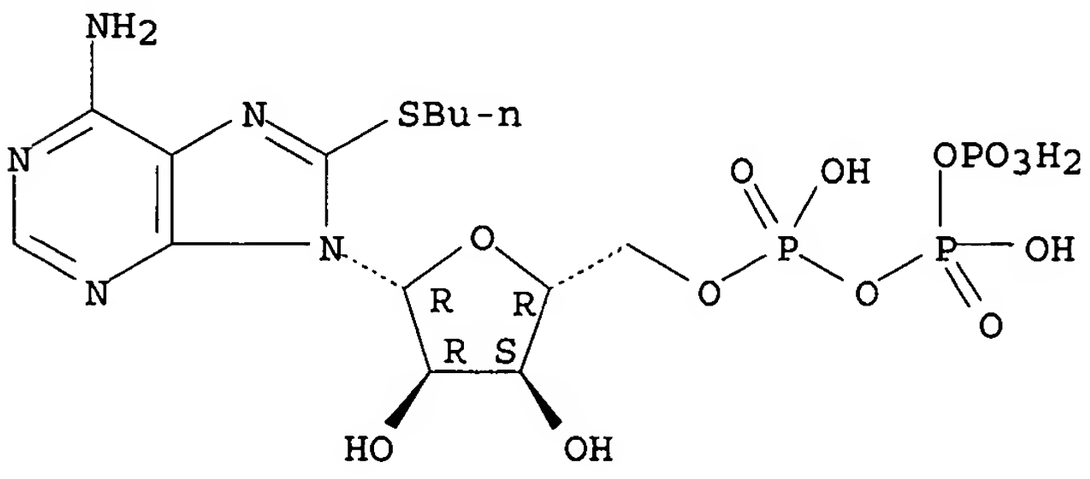
PB American Chemical Society
DT Journal
LA English
AB To elucidate the physiol. role played by nucleoside triphosphate diphosphohydrolase (**NTPDase**; EC 3.6.1.5), adenine nucleotide analogs, modified on the purine ring, have been synthesized and tested as potential inhibitors. Resistance of ATP analogs to hydrolysis and their potency as **NTPDase** inhibitors were evaluated. For this purpose, a particulate fraction isolated from bovine spleen was used as the enzyme source. Among the synthesized analogs, 8-thiobutyladenosine 5'-triphosphate (8-BuS-ATP) was found to be the most effective nonhydrolyzable competitive inhibitor, with an estimated Ki of 10 μM. This nonhydrolyzable analog did not exert any P2X-receptor-mediated effect on endothelium-denuded blood vessels, from the guinea pig mesenteric bed. In agreement with this observation, infusion of the analog did not cause any significant blood pressure variations of the precontracted vessel. Because in previous studies on isolated turkey erythrocytes and rat astrocytes 8-BuS-ATP was not able to trigger any P2Y1-receptor-mediated effect, it therefore appears that this **NTPDase** inhibitor does not interfere with purinergic receptors.
IT **284040-53-5 284040-54-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(synthesis and biochem. and pharmacol. characterizations of novel inhibitors of nucleoside triphosphate diphosphohydrolases)
RN 284040-53-5 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(hexylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 284040-54-6 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(butylthio)- (9CI) (CA INDEX NAME)

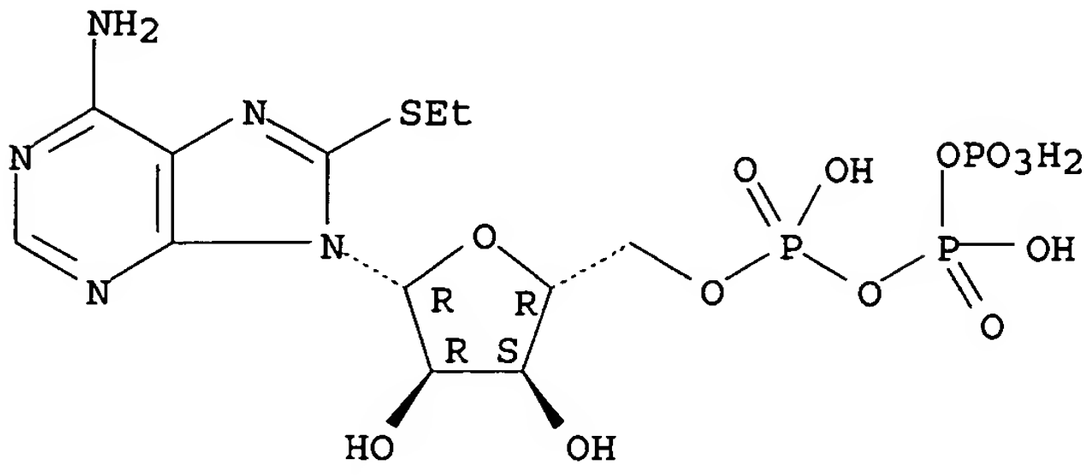
Absolute stereochemistry.



IT **81609-35-0P 284040-51-3P 284040-52-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biochem. and pharmacol. characterizations of novel inhibitors of nucleoside triphosphate diphosphohydrolases)

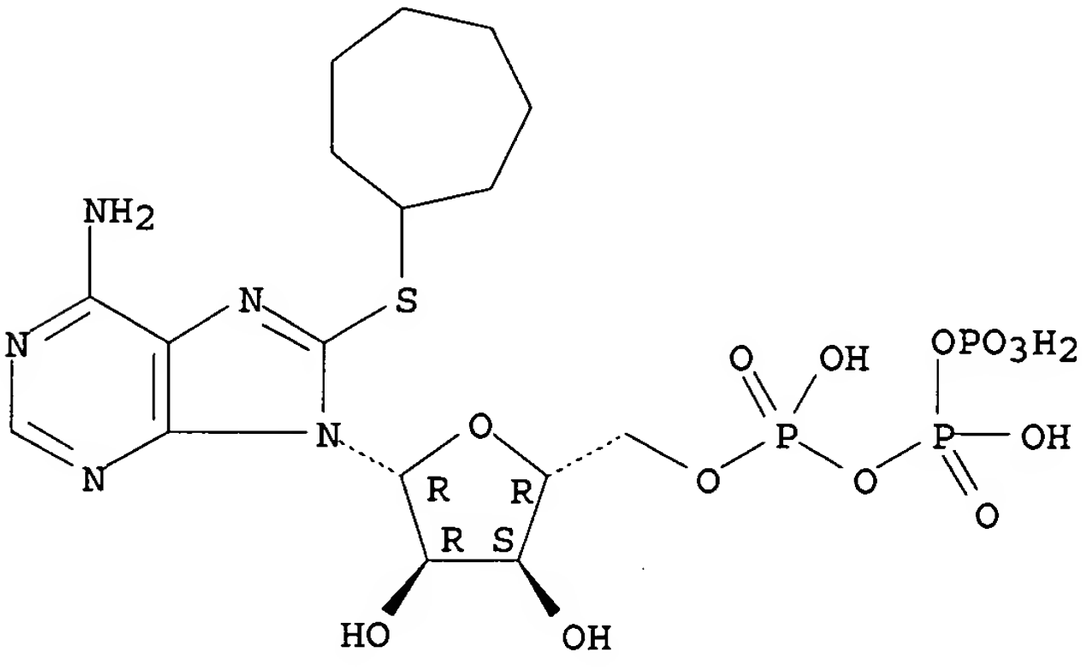
RN 81609-35-0 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(ethylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



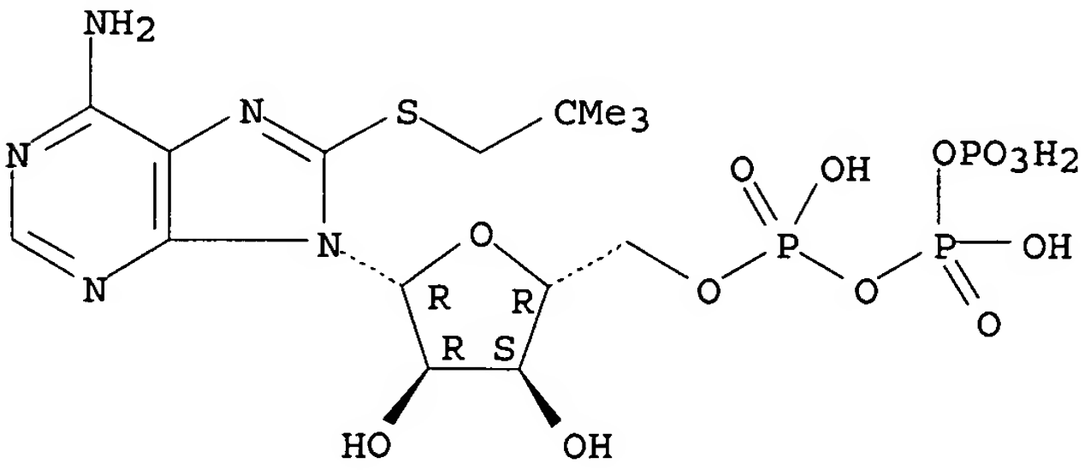
RN 284040-51-3 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-(cycloheptylthio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 284040-52-4 CAPLUS
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-[(2,2-dimethylpropyl)thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT